DESIGN AND SIMULATION OF METHANOL PRODUCTION BY CO_2 UTILIZATION

BY

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A Thesis Presented to the
DEANSHIP OF GRADUATE STUDIES

KING FAHD UNIVERSITY OF PETROLEUM & MINERALS

DHAHRAN, SAUDI ARABIA

In Partial Fulfillment of the
Requirements for the Degree of

MASTER OF SCIENCE

In

CHEMICAL ENGINEERING

December 2018

KING FAHD UNIVERSITY OF PETROLEUM & MINERALS

DHAHRAN- 31261, SAUDI ARABIA

DEANSHIP OF GRADUATE STUDIES

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Dedication

To My Parents,

To my cousin soul wish God bless his soul and makes the rest paradise, and gather us there

my family,

Thanks for every word to supporting me for you pray my father, my mother and my sisters. I dedicate this work to all of you

ACKNOWLEDGMENTS

From the beginning to the end, from the word ‘GO’, and through every high and low in the period of this thesis, a lot of remarkable unpresented gentlemen had helped and guided me to overcome everyday challenges and obstacles, to accomplish the desired mission of producing a meaningful piece of work. To whom, a word of thanking is not even enough to express the amount of gratitude they deserved.

Firstly, I want to thank God almighty for providing me with strength, knowledge, and patience to complete my degree. Secondly, I want to thank KFUPM especially Chemical Engineering Department to give me an opportunity to join the graduate program.

I acknowledge, with gratitude, my debt of thanks to my supervisor, *Dr. Umer Zahid,* for his warm encouragement and thoughtful guidance. I also want to express my deeply-felt thanks to the committee members of my dissertation, *Dr. Eid Mussad Al-Mutairi, and Dr. Mohammed Ba-Shammakh* for their insightful comments, and hard support.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

AD	Alternative Design
AGR	Acid Gas Removal
CCU	Carbon Dioxide Capture Unit
DME	Di-Methyl Ether
GHG	Green House Gases
GTL	Gas to Liquid
HHV	High Heating Value
IEA	International Energy Agency
LHV	Low Heating Value
LPG	Liquefied Petroleum Gas
MEOH	Methanol
METBE	Methyl Tert-Butyl Ether
MM	Million
MMSA	Methanol Market Services Asia
MTO	Methanol to Olefins
MTP	Methanol to Propylene
NG	Natural Gas
PFR	Plug Flow Reactor
PO	Partial Oxidation
RWGS	Reversed Water Gas Shift
SG	synthesis Gas
SN	Stoichiometry Number

SR	Steam Reforming
VR	Vacuum Residue
W.h	Watt per hour
WGS	Water Gas Shift

ABSTRACT

Full Name : [SIDDIG SEEDAHMED SIDDIG KHALAFALLA]

Thesis Title : [INTENSIFIED PROCESS DESIGN FOR THE INTEGRATED METHANOL AND POWER PLANT]

Major Field : [CHEMICAL ENGINEERING]

Date of Degree : [December 2018]

The demand for cleaner and alternative energy is growing rapidly leading to interest in methanol production. Methanol is a high value chemical that serves as an intermediate for producing common chemicals, use as a fuel additive, and as a method of energy storage. This work is about a design of a methanol production plant from coal through gasification technology.

This study presents a simulation model for converting coal to methanol, based on gasification technology with the commercial chemical process simulator, ASPEN PLUS V9.0. The methanol plant consists of air gasification unit, gas clean-up unit, water gas shift unit and methanol synthetic unit. The clean synthesis gas is produced with the first and second operating units (gasification and acid gas removal units). Clean syngas goes through feed preparation unit to reach the reaction requirements. Adiabatic plug flow reactor used to produce methanol and fed to purification section to get desired purity over 98.7 wt.%. Three different alternative design have been developed. AD2 shows it has best performance in terms of energy consumption, CO_2 emission and it in the same range in the cost per production and have value of 9.7 MW.hr/ton Methanol, 88.9 ton CO_2 /year and 166.4 $/ton methanol respectively. The result shows that the methanol synthesis from coal through gasification technology is feasible.

ملخص الرسالة

الاسم الكامل: صديق سيد أحمد صديق خلف الله

عنوان الرسالة: تصميم عملية انتاج الميثانول والطاقة المتكامل

التخصص: هندسة كيميائية

تاريخ الدرجة العلمية: ديسمبر ٢٠١٨

يتزايد الطلب على الطاقة النظيفة والبديلة بسرعة مما يؤدي إلى الاهتمام بإنتاج الميثانول. و الميثانول عبارة عن مادة كيميائية عالية القيمة تستعمل كوسيط لإنتاج مواد كيميائية شائعة ، واستخدامها كمادة اضافية للوقود ، وكطريقة لتخزين الطاقة.

يدور هذا العمل حول تصميم مصنع للميثانول من الفحم عبر تكنولوجيا تحويل الغازثاني اوكسيد الكربون.تعرض هذه الدراسة نموذج محاكاة لتحويل الفحم إلى ميثانول ، استناداً إلى تقنية المحاكة للعمليات الكيميائية باستخدام برنامج ASPEN PLUS V9.0. يتكون مصنع الميثانول من وحدة تحويل الفحم الى غاز عنطريق الاحتراق غير الكامل ووحدة معالجة الغازالناتج من الشوائب ووحدة تبديل غاز الى هايدوجين ووحدة تصنيع الميثانول. يتم إنتاج الصطناعي الخالي من الشوائب والمواد الغير مرغوب فيها من خلال وحدات التشغيل الأولى والثانية. يمر الغاز االاصطناعي بعد المعالجة من خلال وحدات للوصول إلى متطلبات التفاعل من ناحية درجة الحرارة والضغط. يستعمل مفاعل دفق ثابت الحرارة يستخدم لإنتاج الميثانول ، يرسل الميثانول الخام إلى قسم المعالجة للحصول على درجة النقاة المرغوبة والمقدرة بحوالي ٩٨,٧٪ بالوزن. تم تطوير ثلاثة تصاميم بديلة مختلفة لتحسين أداء العملية من نحاية استهلاك الطاقة وانبعاثات غاز ثاني اوكسيد الكربون من العملية . يوضح التصميم البديل الثاني أنه يتمتع بأفضل أداء فيما يتعلق باستهلاك الطاقة ، وانبعاثات ثاني أكسيد الكربون ، وفي نفس الوقت من حيث تكلفة الإنتاج ، وله قيمة ٩,٧ ميجاواط / ساعة / ميثانول ، و ٨٨,٩ طن CO_2 / سنة ، و ١٦٦,٤ دولار / طن. الميثانول على التوالي. تظهر النتائج أن تصنيع الميثانول من الفحم من خلال تقنية تحويل الفحم الى غاز ممكنة ن الناحية العملية والناحية الاقتصادية.

CHAPTER 1

INTRODUCTION

1.1 Background

In the 20th century humanity has rapid increasing in population also there is an explosive growth in energy consumption. New technologies and man-made products started a new era of which one of the most revolutionizing was that of transport, namely the invention engine powered planes, cars, ships and train. This has made the world totally dependent on the combustion of hydrocarbon fossil fuels, such a LPG, gasoline and diesel. Also, the invention of electrical power plants and electric appliances has made us increasingly dependent on fossil fuels such as coal and natural gas. Currently 85% of the world's energy comes from fossil sources. This unprecedented era of development fueled by fossil-based carbon has led to environmental problems that mankind has started to become consciously aware of in the last few decades. The most problem is global warming. [1 – 3].

Greenhouse gases emission Increased that leads to global climate change, affecting humans as well as other species animals and plants. Most greenhouse gas emissions are related to the combustion of fossil fuels to produce power as it shown in figure 1.1. Another problem regarding fossil feedstock is that we are often threatened with depletion of them. The lack

of oil affects both the energy security around the world and the availability of feedstock used in the chemical industry.

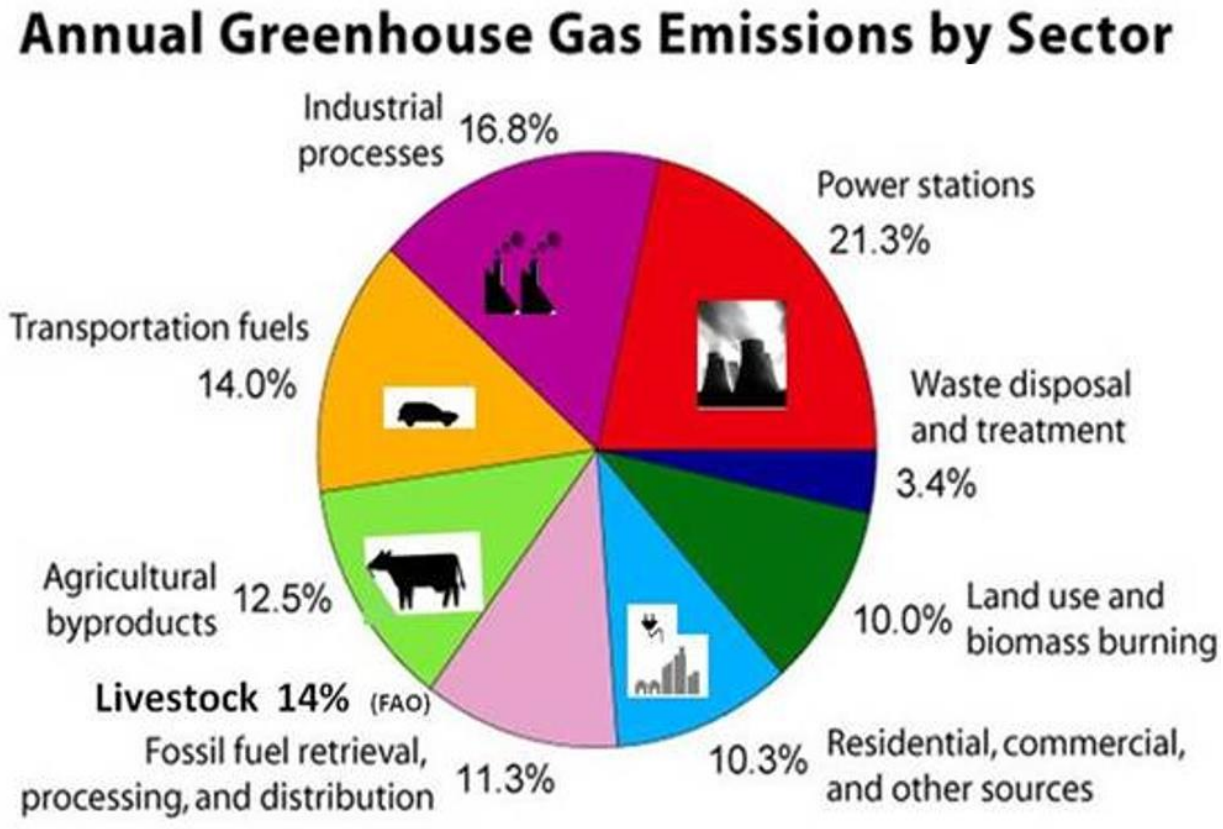

Figure 1-1: Greenhouses gases emissions.[4]

Facing the global warming associated climate change one of the biggest challenge is to continue being able to cover the global energy required while as the same time reducing the dependency of the fossil fuels and reducing the emission of greenhouse gases (GHG's) as decided upon in the Paris Agreement [5]. Figure 1.2 shows that this problem becomes more complex and the energy demand is increasing [6]. To achieve the goals of the Paris agreements, a move towards green energy sources needs to happen. One example of the green energy is renewable energy sources such as solar, wind and biomass. The main

challenge is check their ability to fill up the deficiency with the human needs and their carbon natural transformation to energy. Hydropower, wind biomass, solar and geothermal energy these are green energy sources that can be used different energy uses such as electricity, fuels and heat.

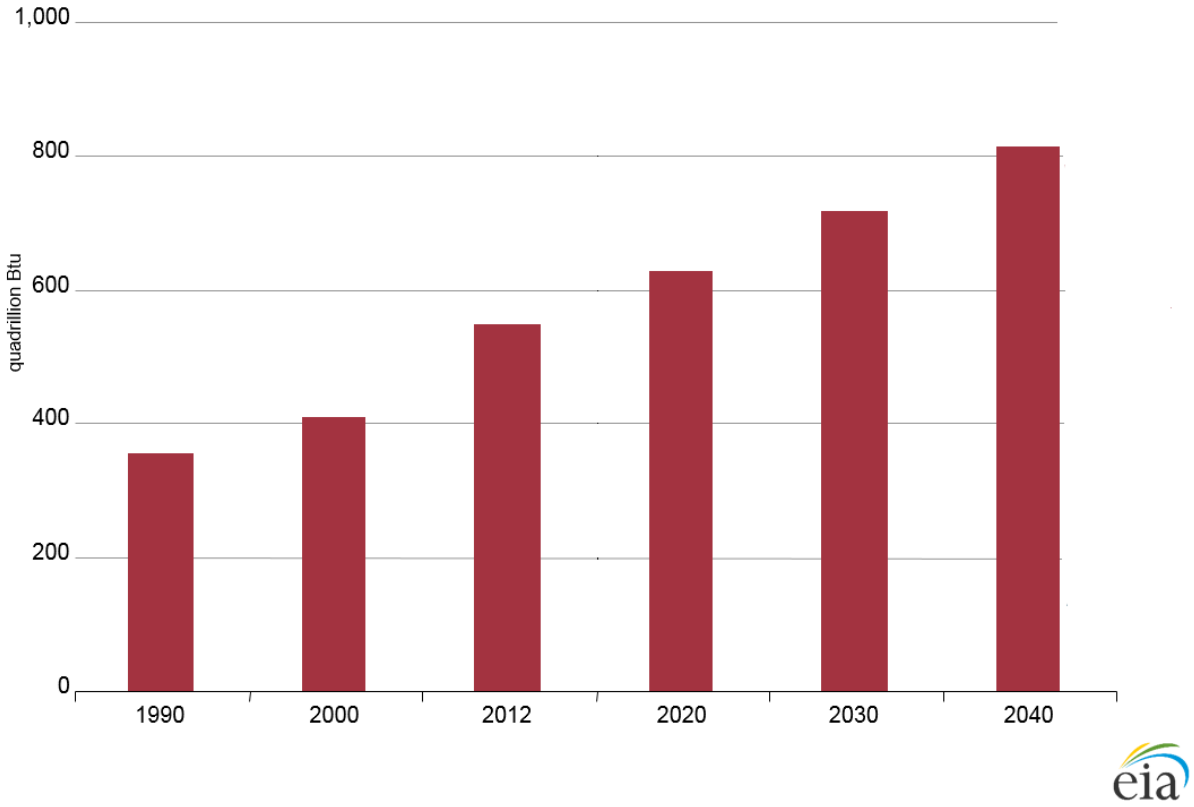

Figure 1-2 Global energy demand in quadrillion BTU.[7]

World economy depends strongly on the sources of the energy and their richness. Globally the annual energy uses in 2012 is about 1.60 thousand tones W.h and it has increased profile from that time with increased percentage 1.2 % annually. Fossil fuels are the main source of energy for centuries due to availability in the world. Due to the restriction of emission

of carbon dioxide and the effect of the Green House Gases (GHG's) and their contribution in the global worming all the world focus on the green energy and one of them methanol [8].

Methanol is simple alcohol with formula CH_3OH that is one of the famous chemical material produced now days due to widely range of the process, which they use it. Methanol has different applications in the industry it can used as solvent or it can feed to produced organic materials such as acetic acid, methyl tert-butyl ether (MTBE) and formaldehyde [9], [10].

Moreover, methanol can be used in the field of energy since it has high caloric value, which made it one of good fuels because it costs less than other alternative fuels and it is an oxygenated fuel, which burns cleaner also it has a higher octane rating, which enhances engine performance and it is safer , and it is one of the friendly environmental fuels which it has lower emission of pollutant comparable with conventional fossil fuels.

Although, di-methyl ether (DME) can be used instead of conventional deasil which it can produced by dehydration of methanol. Finally, it can be as feedstock for a bio-fuels production [11].

The global production capacity of methanol with an average 10% since 2009, while the production has been increasing slightly smaller rate around 7% till reaching around 60.6 mega ton according to Methanol Market Services Asia (MMSA)or about 58 mega ton in 2012 according to International Energy Agency (IEA). On the other hand, the global methanol demand is driving the growth in production and it depends on the main derivative

demand, which is expected to increase in the next five with an average reach 5% that illustrate in figure 1.3. [12].

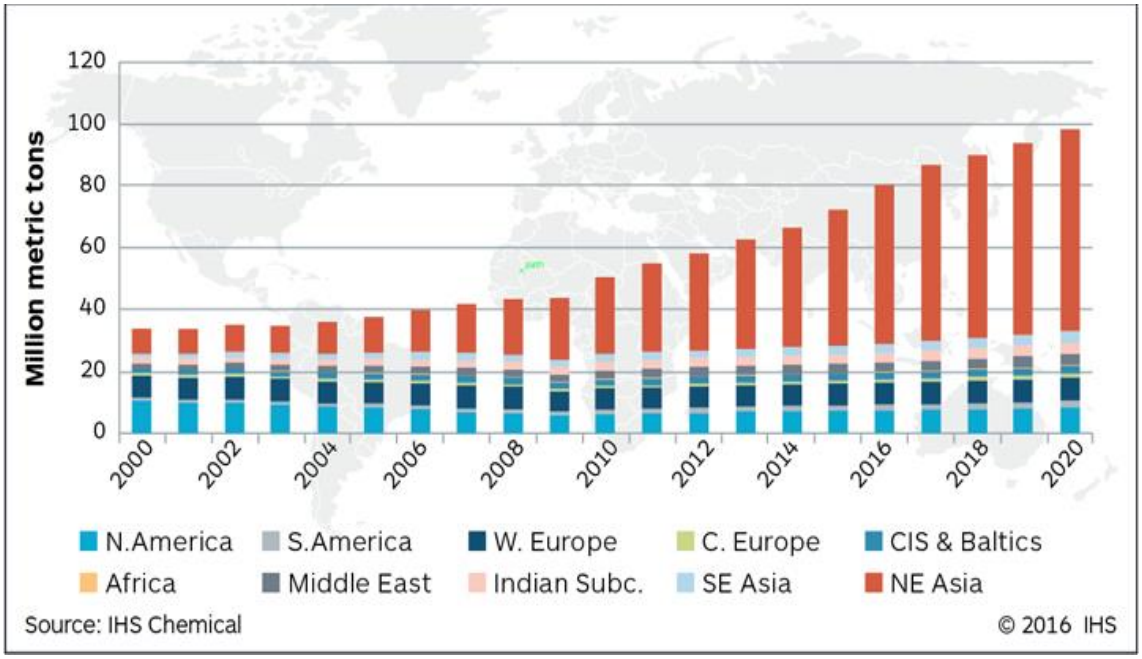

Figure 1-3: Methanol Market over the world.[13]

China leads the methanol market and it is the largest methanol consuming country, owing to increasing in demand of methanol, it is essential to optimize the various available processing technologies and made it more economically. Efforts to upgrade the technology and to incorporate latest research developments in methanol production process since its implementation in 1923 [14].

Since methanol is very important chemical intermediate that it has different applications convert it into useful products and merchandise. The demand of methanol in terms of end uses over the world could be illustrated in Figure 1-4.

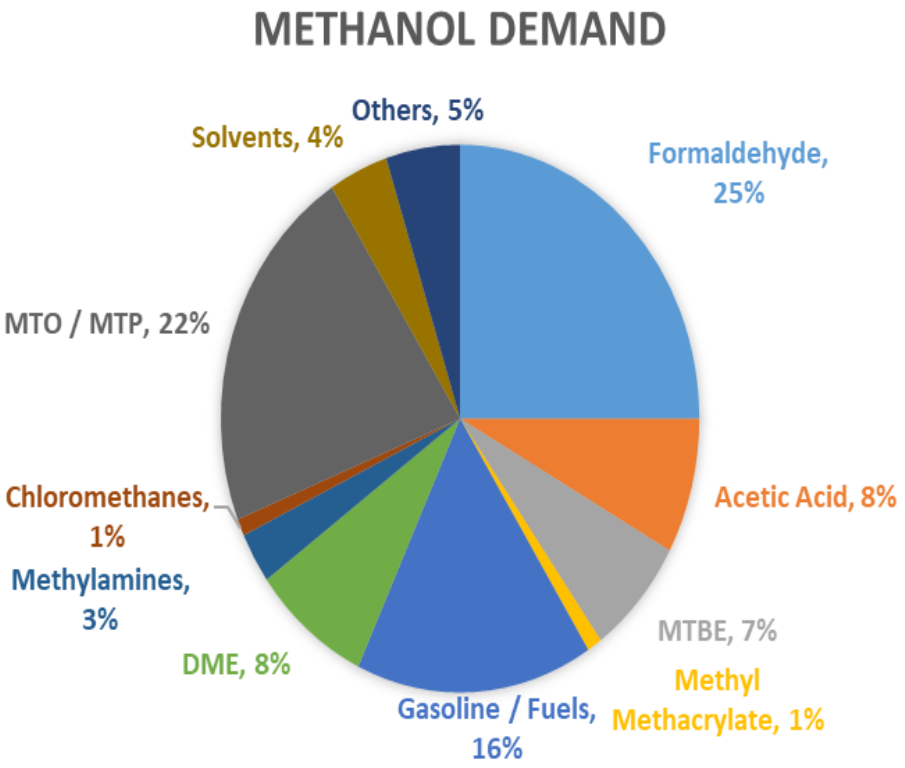

Figure 1-4: Methanol demand based on uses.[13]

Formaldehyde production process had the major contributor of methanol consumers, accounting for almost 25% of methanol global demand that is equal to 92.3E+6 tons. Gasoline or Fuel applications consume about 16%. The consumption of methanol into direct fuel applications surpassed MTBE as the second largest market for methanol, with almost 7% of global methanol demand. MTBE and Acetic acid anhydride each share 10% of methanol market volume. Methanol to Olefins (MTO) and methanol to propylene (MTP) demand is anticipated to become a high growth sector share 22%. Other uses of methanol include wastewater de-nitrification, hydrogen carrier for fuel cells, transesterification of vegetable oils for biodiesel production and electricity generation. There are thousands more products that also touch our daily lives in which methanol is a key component [15].

Methanol is an energy carrier it is not an energy source, it has high heating value of approximately 23 MJ/kg. The energy content for methanol is almost half of common transportation fuels like gasoline and diesel as shown in table 1.1. On the other hand, it has high octane number becauses of the mileage of ICE-driven vehicle comparable to conventional fuels, due to higher compression ratios. Especially for the transportation sector, the major issue is an energy carrier problem not an energy problem [16].

Table 1-1: Different types of fuels with their heating values.

Fuel	**HHV**	**LHV**	**Density**
	MJ/kg	*MJ/kg*	*kg/m^3*
Methanol	22.9	20.1	794
Dimethyl ether (DME)	31.7	28.9	665
Ethanol	29.8	27.0	789
Conventional Gasoline	44.9	44.9	745
Conventional Diesel	46.5	43.4	837
Fisher-Tropsch Diesel	45.5	43.2	797

Methanol is typically produced from several sources like synthesis gas, biomass and natural gas (NG) which is a better choice for methanol production feedstock. Natural gas is preferred as the feed for the process due to its abundance and its environmental friendliness. Several other processes benefit economically from having NG as a feed. Namely, dimethyl ether and synthetic fuels manufacturing from NG using gas to liquids (GTL) processes which is not feasible by conventional means. Natural Gas, a widely used fossil energy source, has estimated proven gas reserves of 177 - 1012 m^3 of which around 40% are not of direct use to the market [17]. The conversion of NG to synthesis gas (SG) and is common in chemical processing plants and it has multiple well-established

technologies. Methanol production has risen by 42% from 2001 to 2008 while the Annual production in 2010 was 45 Mt [18].

1.2 Novelty of the thesis

The novelty of this study to design and develop a novel process of methanol production using Aspen Plus to simulate a process where we utilized coal to produce green energy that has low carbon content by synthesizing methanol. After the process simulation complete, a complete economic evaluation and energy analysis in order to evaluate its applicability in large scale. Further analysis study to check the sustainability and alternative design have been studied to evaluate the best way and to improve the process and minimize the cost.

1.3 Structure of the Thesis

This thesis is written and organized in the form of Chapter-based thesis. Each chapter discussed below.

Chapter 1 gives abackground to methanol uses, market of methanol and demand of the methanol over the world. Also, it discusses the novelty of this these and what is the contribution.

Chapter 2 presents the literature review for the topic and what is the process to process the methanol and how could the synthetic gas produce.

Chapter 3 deals with methanol synthesis process flowsheet that was developed and fully description for the process and discussed the alternative process which are developed.

Chapter 4 presents the process simulation and the main parameter used to develop the model.

Chapter 5 discuss the main process stream results, the energy performance for the base case and the alternatives, the carbon dioxide emissions from the process and the economic study that consist from the capital cost, operational cost and the cost of unit produced.

Chapter 6 shows the conclusion from this work and what is the recommendations.

CHAPTER 2

LITERATURE REVIEW

In this part syngas production and methanol production will be studied and some process studies will be mention.

2.1 METHANOL PRODUCTION

Methanol is important for the future energy and fuel industry feedstock as well as for the chemical industry. The current globally installed production capacity of methanol is around 110 billion metric tonnes per year [19] to meet the demand of 70 billion metric tonnes. At the moment mostly, all methanol is produced from natural gas through reforming and catalytic conversion. However, the use of coal and other feedstock for syngas generation is being researched and implemented. The change of feedstock is supported by the similarity of syngas produced from natural gas and from another feedstock.

2.1.1 Conventional methanol production process

Catalytic conversion of synthesis gas which is gaseous mixture of CO, CO_2 and H_2 is the most common method to produce methanol industrially. Various carbonaceous components could also be used to produce methanol.

$$CO + 2H_2 \leftrightarrow CH_3OH \ , \Delta H_{298K} = -91 \frac{kJ}{mol} \quad (2.1)$$

$$CO_2 + H_2 \leftrightarrow CO + H_2O \ , \Delta H_{298K} = 41 \frac{kJ}{mol} \quad (2.2)$$

Equation 2.1 is highly influenced by thermodynamic factor such like thermodynamic equilibrium which effect the process that it gave low conversion per pass therefor large unreacted gas recycled back to reactor. The reaction is extremely exothermic there for significant cooling duty required.

The ideal stoichiometry for syngas ratio H_2 /CO is equal to two as suggested by Equation 2.1

Also, there are another parameter effect the production which called stoichiometry number also called as module (M) which defined as the Equation 2.3. on the following page [20].

$$M = \frac{x_{H_2} - x_{CO_2}}{x_{CO} + x_{CO_2}} \approx 2 \qquad (2.3)$$

In1923, BASF made the first commercialised technology based on Zn-O-Cr_2O3 catalyst that could produce methanol from hydrogenation of CO at 350- 400 ^oC and 240-300 bar. In 1960, A major improvement achieved by ICI which Cu/Zn-O catalyst was used which has good performance and could work under much lower operating condition 250 - 280 ^oC and 60-80 bar.

Recently, to avoid large gas recycle various schemes for once-through operation have been conceived .Some of them based on multiple reactors placed in series with inter-stage removal of methanol, by deferent process of separation like absorption in an liquid, by reactive chromatography condensation or Condensation .Other schemes methanol removed inside the synthesis reactor by means of a using solid adsorbent particles or liquid absorbent, by means of methanol condensation or means of a methanol permeating membrane [21].

Most of these once-through schemes supernumerary the large energy duty of the gas recycle loop by other large transfer duties. Such as, the use of liquid absorbent and solid adsorbent] require regeneration of the absorbent or adsorbent. The series scheme of van Dijk and Fraley [22] required inter-stage cooling. Removal of methanol by condensation or by membrane doesn't has high energy consumption. However, still it has some limitations. One of the Limitation of membrane reactor is expensive to construct at large scale. However, for the condensation reactor the low operation condition implies low volumetric productivity which expect to have a large and costly reactor.

2.1.2 Methanol production from carbon dioxide

Methanol could be produced from other feed source. One of the other sources is carbon dioxide CO_2. There are two different way to produced methanol from CO_2; either it can be one step or two steps. One Step is directly hydrogenation of CO_2 as it mentions in Equation 2.3.

$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O, \Delta H_{298K} = -87 \frac{kJ}{mol} \quad (2.4)$$

For the two steps, the CO_2 is converted to CO with the reaction in Equation 2.2 which is called Reversed Water Gas Shit (RWGS) reaction which in turn is a very important industrial reaction that produces hydrogen and then hydrogenation to produced methanol. CO_2 had different routes to produce useful material which is mentions in figure 2.1 [11], [23], [24].

$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O, \Delta H_{298K} = -87 \frac{kJ}{mol} \quad (2.5)$$

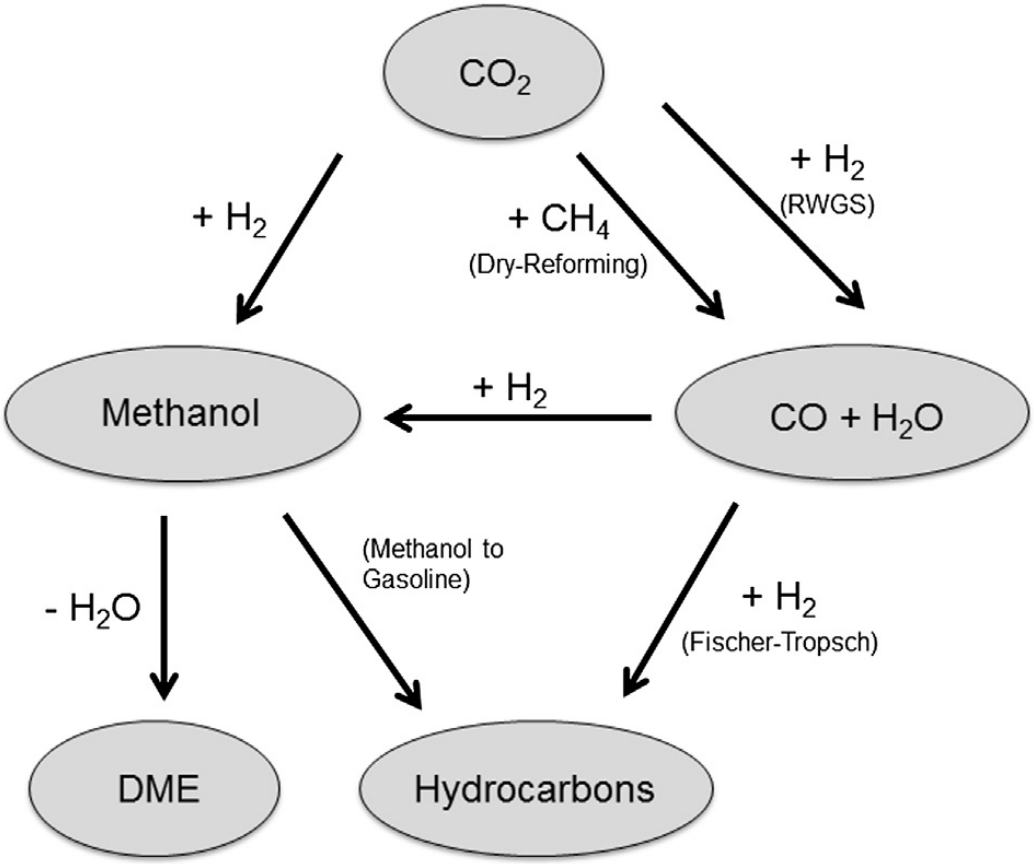

Figure 2-1: The routs for CO_2 utilization.

The production of methanol from CO_2 hydrogenation has been extensively studied. Joo et al. (1999) concluded that production of methanol has a higher yield for two step process compared to one step process [25][26].

Mignard et al. (2003) proposed a methanol synthesis process from CO_2 captured from flue gas of a coal power plant and electrolytic hydrogen [27]. The process requires the utilisation waste heat in the power plant to provide thermal energy to achieve a significant reduction of CO_2. In the absence of thermal sources, CO_2 abatement is almost non-existent .

According to Mignard and Pritchard (2006), The methanol process showed the highest energy efficiency compared to other production processes (methanol, ethanol and gasoline from the CO_2 hydrogenation) [28]. Pontzen et al. (2011) carried out experiments to compare the production rates methanol from CO2 over Cu-ZnO/Al_2O_3 catalyst with the conventional syngas production processes [29].

The CO_2 based process displayed lower production rates in comparison to the conventional one. Soltanieh et al. (2012) conducted the economic analysis the co-production of methanol and electricity from carbon-free hydrogen and captured CO_2 [30].

Van Der Ham et al. (2012) designed a fluidised-bed membrane reactor for CO_2 to methanol conversion process . It showed significant CO_2 reduction, however, it did not satisfy economic viability [31].

2.2 Synthesis gas production

The Syngas is the gas that consist of carbon mono oxide and hydrogen and it could be produced from different feedstocks that it mentions below.

2.2.1 Syngas production from natural gas

This process it has a lot of impurities that needs to be removed before converted natural gas to synthesis. One of the most important impurities are sulphur component because their effect in posing the catalysts in the downstream processes. There is different process to produce syngas from the natural gas such as steam reforming (SR), partial oxidation (PO), two step reforming and dry methane reforming (DMR) that it will be described clearly with more detailed in the following section the different between some process presented in table 2.1.[32]

2.2.1.1 Steam reforming:

The conventional method is through steam reforming where natural gas and steam is mixed at high operating condition and in the present of catalysts form syngas as Equation 2.6 illustrate.

$$2CH_4 + 2H_2O \leftrightarrow 2CO + 6H_2, \Delta H_{298K} = 205.52 \frac{kJ}{mol} \qquad (2.6)$$

The synthesis gas production is highly endothermic and requires a huge amount of thermal energy.

2.2.1.2 **Partial oxidation:**

Another Method for syngas production is partial oxidation developed in the 1950s by Shell [22].

$$CH_4 + 0.5\ O_2 \leftrightarrow CO + 2\ H_2, \quad \Delta H_{298K} = -36 \frac{kJ}{mol} \tag{2.7}$$

$$CO + 0.5\ O_2 \leftrightarrow CO_2 \quad , \quad \Delta H_{298K} = -283 \frac{kJ}{mol} \tag{2.8}$$

$$H_2 + 0.5\ O_2 \leftrightarrow H_2O, \quad \Delta H_{298K} = -241.52 \frac{kJ}{mol} \tag{2.9}$$

The partial oxidation process for natural gas is to some extent exothermic. The reaction occurs in vapor phase via radical reactions with in flame of burner. To bring up the temperature to the desired 1000-1200 °C Therefor; an excess amount of oxygen is needed to have some oxidation to carbon dioxide and water [33], unfortunately; the stochiometric number drops to 1.6 which is below the optimal case which is equal to 2. Which it is happened due to production of carbon dioxide and water but there is an improvement over steam reforming.

Air separation process is expensive process that it has high contribute in the cost. But it is possible to use air which there is modern plants use it however, it is needed separation unit to be spilt the nitrogen from the synthesis gas after oxidation step.

2.2.1.3 Two-step reforming:

This process is a combination of partial oxidation and steam reforming which it is improve the overall process efficiency and it has better control the composition of the produced synthesis gas. The composition of the natural gas is main factor to define system configuration for the used as feedstock. Two steps reforming requires high enough methane content that is due to steam reforming reacts with high methane slip, around 35-45% and the remains methane needed for partial oxidation [34].

2.2.1.4 Dry reforming:

The reaction between carbon dioxide and the natural gas to synthesis gas called dry reforming.

$$CH_4 + CO_2 \leftrightarrow 2\,CO + 2\,H_2, \quad \Delta H_{298K} = 247.3\,\frac{kJ}{mol} \tag{2.10}$$

Dry reforming is more endothermic reaction compared to steam reforming. moreover, the synthesis gas produced has significant hydrogen that is deficit for methanol synthesis. However, this composition is right for other application.

Table 2-1: Different Reforming process and specification.

	Steam Reforming	Partial oxidation
Type of process	Endothermic	Exothermic
system complexity	complex	very simple
out let hydrogen content	70-80%	35-45%
carbon yield	9% CO	19 % CO
	15% CO2	1% CO2
System configuration	complex	Simple
M	≈3	≈1.8

2.2.2 Synthesis gas production from Coal

Syngas could be produced from coal through a process called gasification. This process is combined between a steam reforming and partial oxidation treatment [35]. The gasification reaction are mentions below.

$$C + 0.5\,O_2 \leftrightarrow CO \quad , \quad \Delta H_{298K} = -123\frac{kJ}{mol} \tag{2.11}$$

$$C + H_2O \leftrightarrow CO + H_2, \Delta H_{298K} = 131\frac{kJ}{mol} \tag{2.12}$$

$$CO + H_2O \leftrightarrow CO_2 + H_2, \Delta H_{298K} = -41\frac{kJ}{mol} \tag{2.13}$$

$$CO_2 + C \leftrightarrow 2\,CO, \quad \Delta H_{298K} = 170.7\frac{kJ}{mol} \tag{2.14}$$

The coal which is used as feedstock is mainly the factor effect the design and process conditions. The produced gas has a deficit of hydrogen and it is related to the water gas shift reaction Equation 2.13 that improve the ratio between hydrogen and carbon

monoxide and it is need purification from sulfur component mainly hydrogen sulfide which it must be removed before methanol synthesis to protect the catalyst from poisoning.

2.2.3 Synthesis gas production from Biomass

Most of alcohol (ethanol and methanol) could be produced from different kind of biomass such as algae, municipal waste, wood and agricultural waste through process called gasification.

Multiple challenges are encountered in the case of production from biomass namely the cost of production. The biomass composition requires high capital investment costs from the production plants inquire despite its lower energy conversion efficiency in comparison to natural gas and coal [36].

Methanol is conventionally produced from biomass is through gasification of the feedstock. A plausible alternative is enzymatic conversion, despite the current focus on ethanol production. In the case of sea growing plants like macro- and microalgae, cattail, water hyacinth etc. good alternative. is anaerobic digestion to produce methane to be used similar to natural gas. Along with enzymatic conversion, further research and development is needed prior to large scale commercial implementation [35].

There are similarities between the gasification process of biomass and synthesis gas production from coal. In the gasification of biomass, the feedstock is dried and pulverized while maintaining the moisture content should below 15-20 wt.%.

Pyrolysis or sometimes it called destructive distillation is the first step in two step gasification. The dried biomass is heated to 400-600 °C in less sufficient amount of oxygen to prevent complete combustion (partial oxidation). The produced gas after gasification is mainly contain carbon monoxide, carbon dioxide, hydrogen, water also there are some volatile tar released. The remaining product called charcoal that in future could be react with oxygen at high temperature to produce carbon monoxide.

The synthesis gas produced from the pyrolysis and charcoal conversion needs some purification processes before it be used in the methanol synthesis.

Biomass has lower content of Sulphur compare to coal. However, it has tar content that effect the process performance and has some operating challenges because it Deposits in the filters pipes and boiler. This issue can be controlled by choosing an optimal process conditions and a right technique according to the composition of the biomass. Partial oxidation could be used as an alternative process rather than the two steps gasification process. However, it has technical challenge to be used for large scale operations.

Synthesis gas production from biomass is conceivable at little scale however at large scale coal and natural gas are favored because of high cost. Large demand of feedstock material is the strategic difficulties for biomass plants however, it has lower energy content compare to coal and natural gas [37].

Moreover, gathering, transportation and storage of biomass it might be one of the biggest obstacles towards the development on large scale plants.

Converting biomass to bio-crude is an alternative proposed to solve the transportation issue that through a fast pyrolysis process that it operates at atmospheric

pressure and 400-600 °C to avoid cracking it produced black fluid and easy to be transported called bio-crude.

CHAPTER 3

PROCESS DESCRIPTION

In this chapter the process description for coal to methanol process will discussed and the alternatives design for the process to enhance the performance of the process and the energy consumption.

3.1 Base case design

Methanol production from coal it should pass through different process first coal should be prepared in the feedstock preparation unit then followed by gasification unit where the synthetic gas produced. Then the produced gas sends to cleaning unit to remove the impurities for the synthesis gas where the CO_2 and H_2S captured there.

The clean gas sends to water gas shift (WGS) unit to convert the syngas to hydrogen using steam and there is CO_2 capture to fix the ratio between carbon dioxide and the hydrogen and to modify the stichometry number to be equal to 2 which the optimum value to produce the methanol. The produced gas fed to methanol synthesis section the block flow diagram for this process illustrate in figure.3.1.

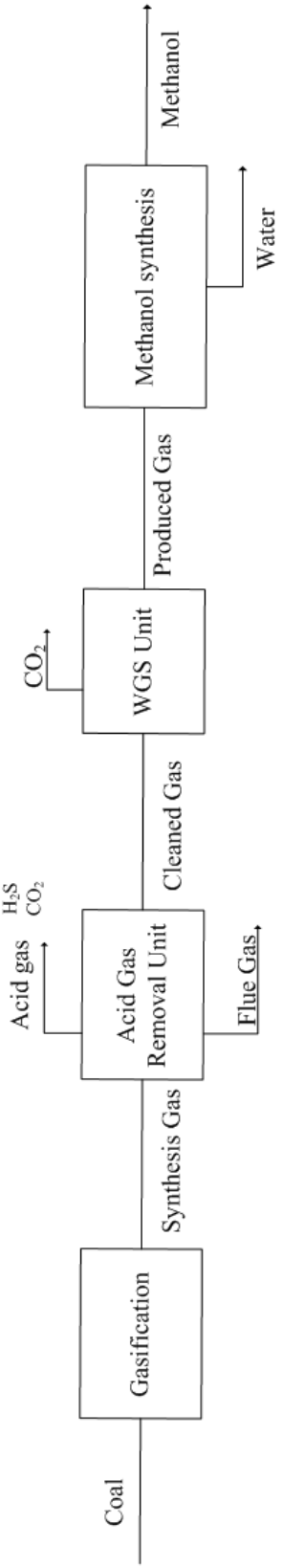

Figure 3-1: Block Flow Diagram of base case.

3.1.1 Gasification unit

This unit consist of two parts preparation feed unit where the coal was mixed with water and crushed to fine particle using two crushers then it sends to screen mesh unit that separate the big size particle from the small size where the big one sends them back to crusher then the prepared coal sends to gasifier part. Preparation feed unit illustrated in figure .3.2.

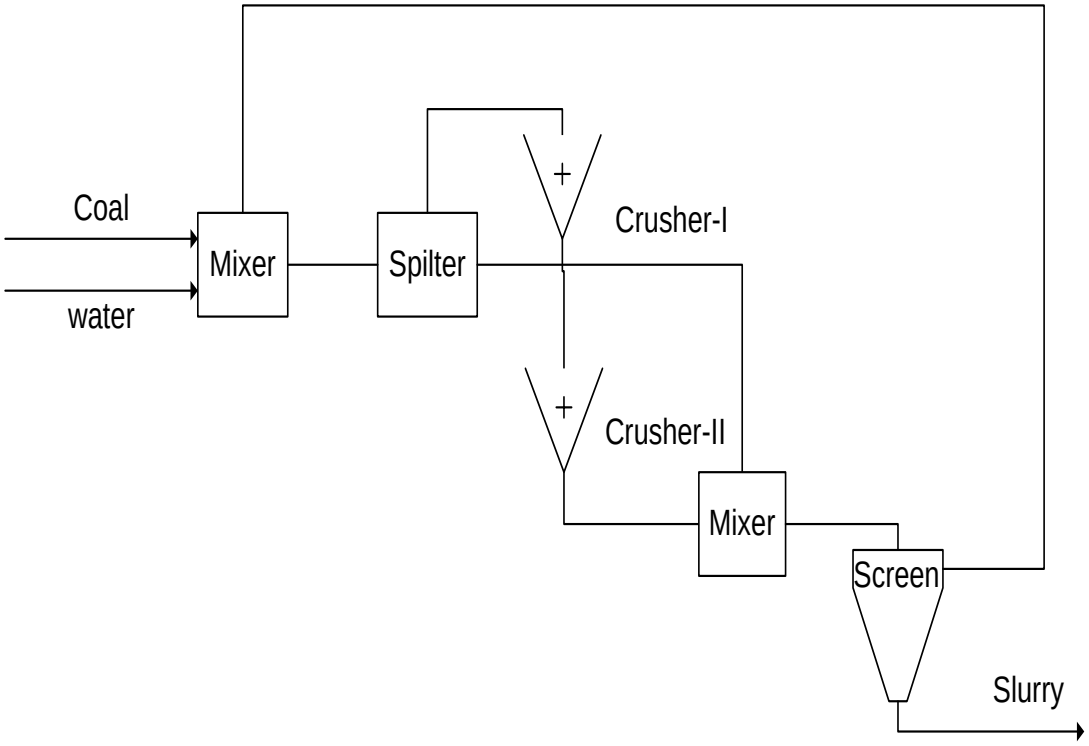

Figure 3-2: Process flow diagram for feed preparation unit.

The prepared coal fed to first reactor (combustion reactor) then it is sends to second reactor (Gasifier) to produced synthesis gas has high temperature which is utilized to produce high pressure steam using boiler. Syngas produced has consist of mainly carbon mono-oxide, hydrogen carbon dioxide and different impurities content such as COS, acid gas and sulphur components. Flowsheet for gasifier section shown in figure 3.3.

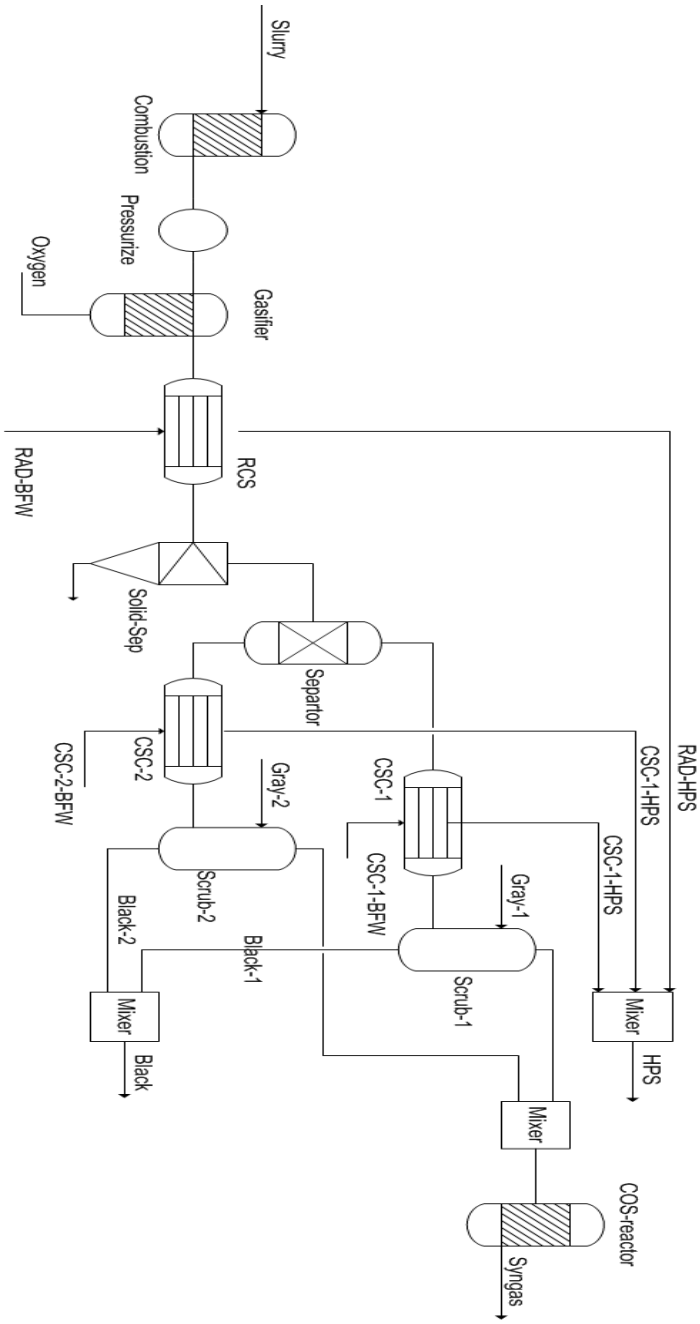

Figure 3-3: process flow diagram for the gasification section.

3.1.2 Acid gas removal unit

The synthesis gas fed to pre-cooler heat exchanger then to gas liquid separation unit to remove condensed liquids, then it fed to the bottom of the absorber unit while the lean solvent fed to top of the column then the syngas contact with the physical solvent (Methanol) the sweet gas and the rich solvent leave the column from the top side and from bottom respectively. The rich solvent fed to regeneration unit (stripper) that separate the acid gas from the solvent then recycle the lean solvent. In this unit there are to contactor in series the first one is to remove H_2S and the second one for CO_2 the process flow diagram for this section shown in Figure 3-4.

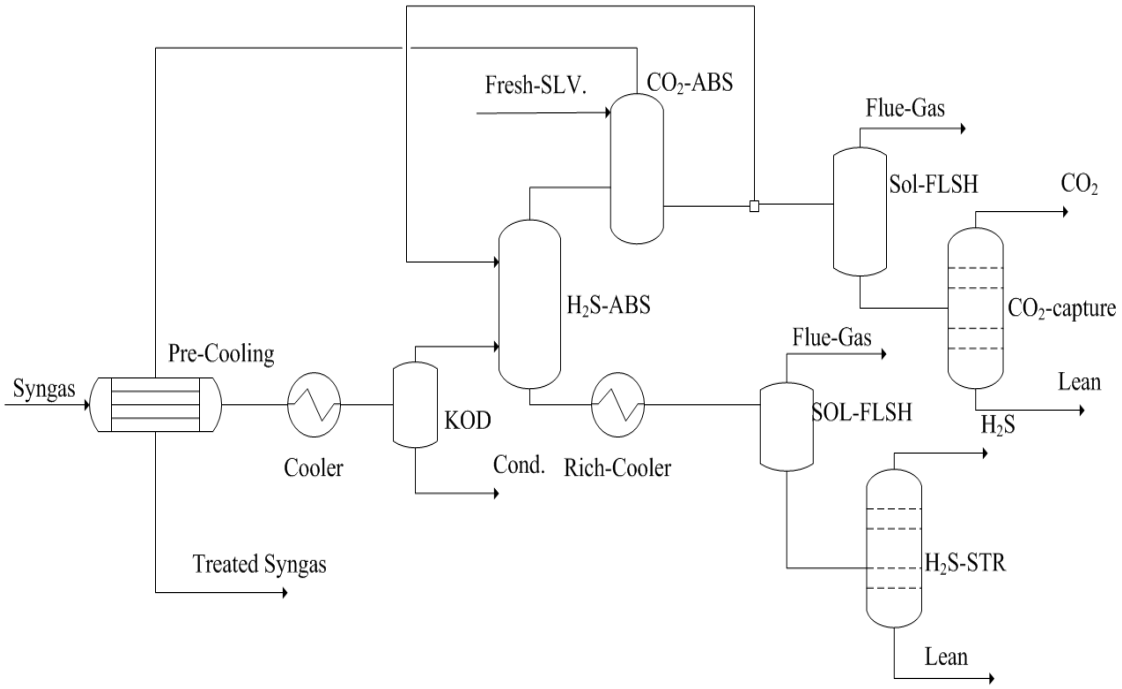

Figure 3-4: Process flow diagram for the acid gas removal unit.

3.1.3 Water Gas Shift unit

The treated syngas after cleaning fed to water two stages shift reactor with intercooling to enhance the hydrogen amount in synthesis gas the it sends to CO_2 cleaning unit to fix ratio for CO_2: H_2 to equal three the process flow illustrates in figure 3.5.

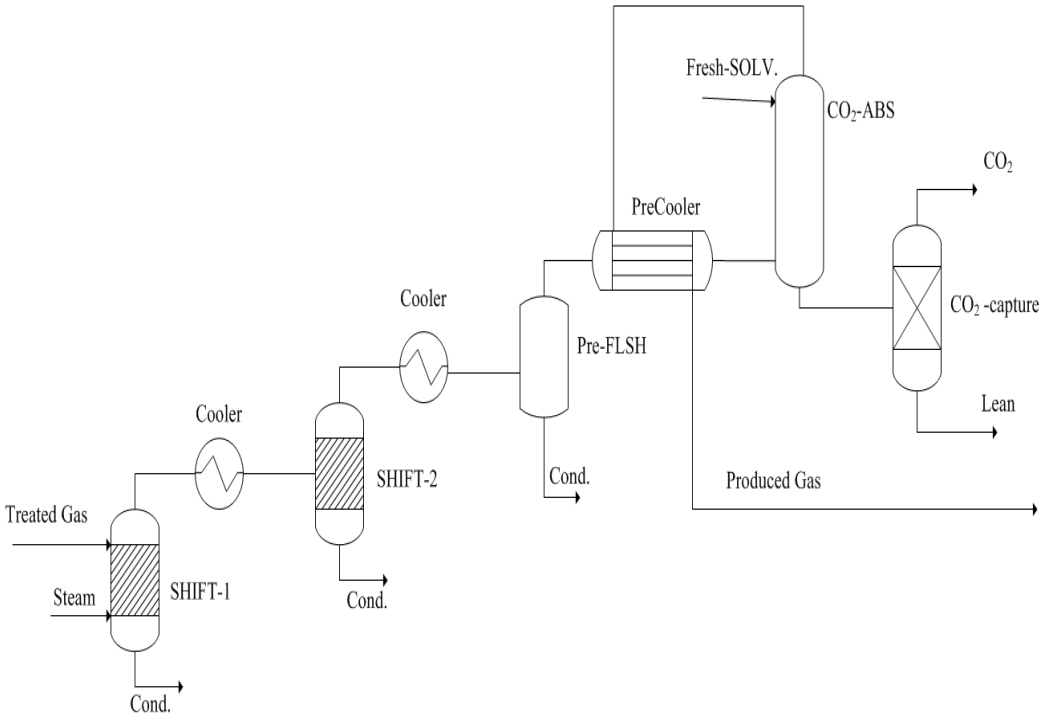

Figure 3-5: process flow diagram for water gas shift unit.

3.1.4 Methanol Synthesis unit

The sifted gas fed to compressor then to preheater then it fed to plug reactor where the methanol is produced using catalytic conversion for CO_2 on ZnO-CuO/Al_2O_3 catalyst. The product cooled then the separated while 99% of unreacted gas recycled back after compressed and heated and the remain had been purged to avoid accumulation of inert gas the liquid product send to low temperature separate to remove off gas then it fed distillation column where the methanol from water the process flow diagram illustrated in figure 3.6 below.

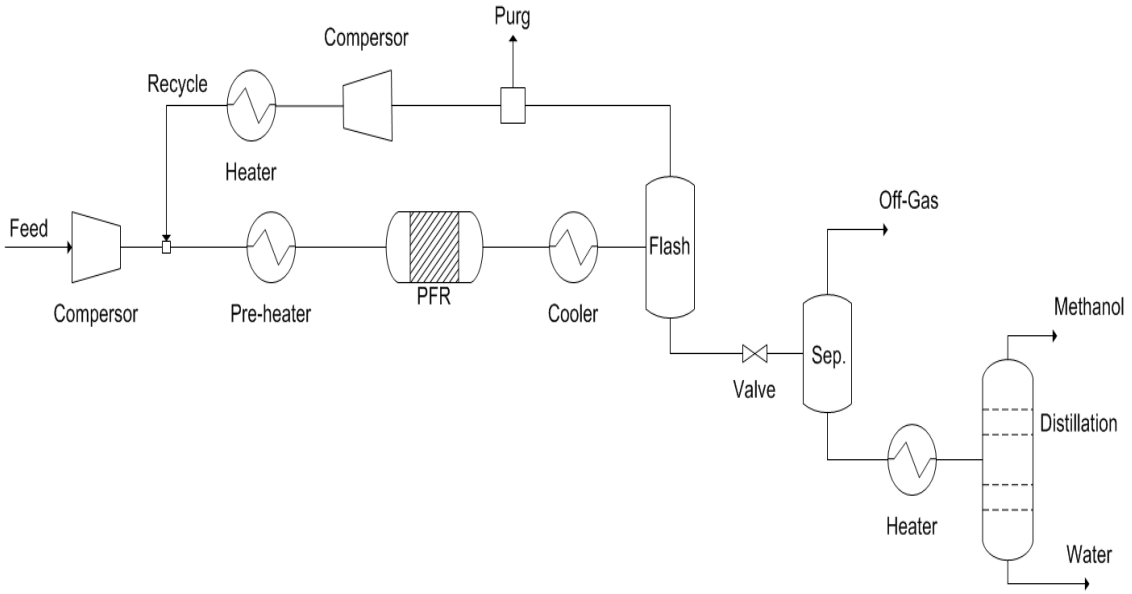

Figure 3-6: Process flow diagram for Methanol synthesis section.

3.2 Alternatives design

Alternative design for the process have been designed to enhance the performance of the process by minimize the energy consumption either to decrease the carbon dioxide emission or the decrease the cost of the plant.

3.2.1 First alternative design (AD1)

Alternative design 1 (AD1) is like the base case design containing gasification, H_2S cleaning unit only, WGS and methanol sections. However, the main difference in the AD1 is the absence of CO_2 cleaning unit. In this case, CO_2 is not removed from the syngas in the WGS unit and it directly fed to the methanol section along with the H_2 gas. The block flow diagram for the AD1 is shown in figure 3.7.

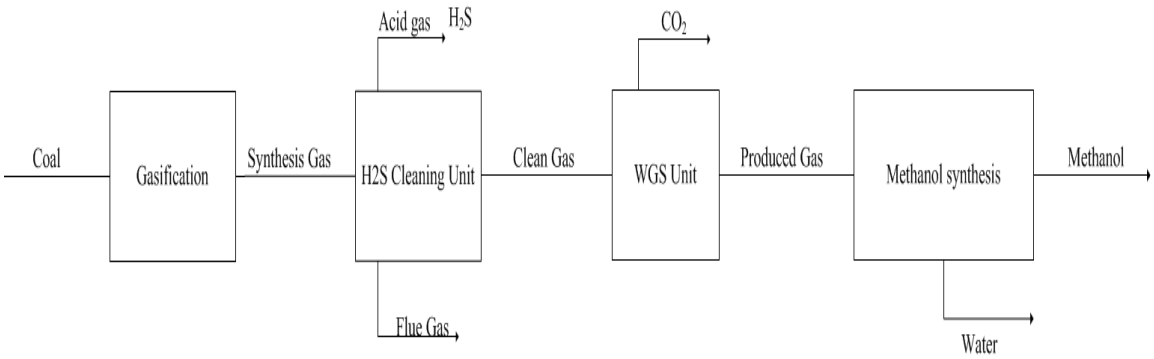

Figure 3-7: block flow diagram for the first alternative.

The modified process flow diagram for the cleaning that in cloud only H_2S cleaning shown in figure 3.8

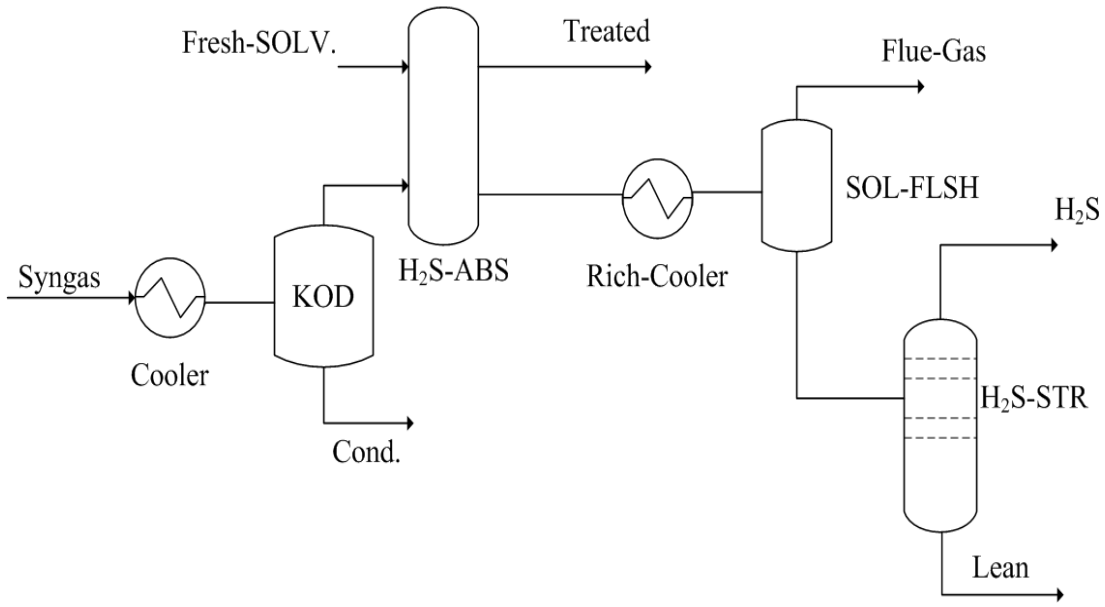

Figure 3-8: Process flow diagram for the H_2S cleaning unit.

3.2.2 Second alternative design (AD2)

The block flow diagram for second alternative design (AD2) is shown in figure 3.9, is like AD1 containing gasification, H_2S cleaning unit only, WGS and methanol sections. However, the main difference in the AD2 from the base case design is the absence of CO_2 cleaning unit in WGS. There for to maintain the ratio for CO_2: H_2 fresh Hydrogen fed to methanol section.

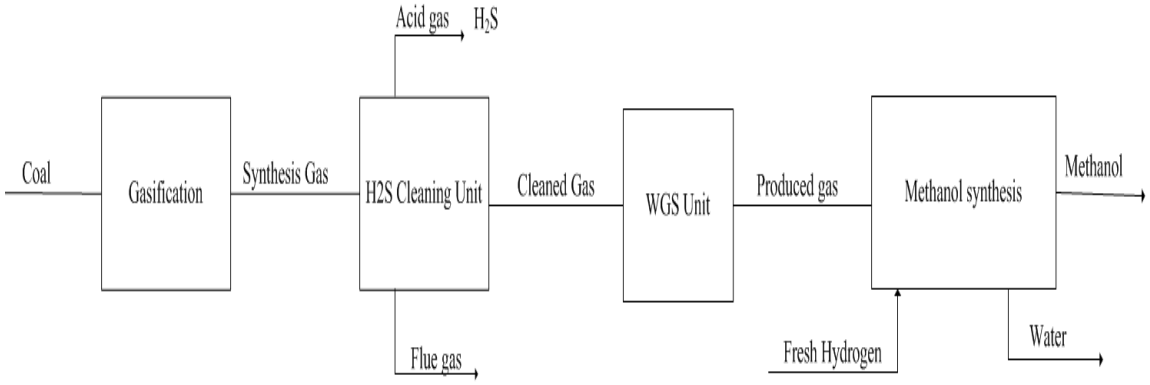

Figure 3-9: block flow diagram for Alternative design 2.

3.2.3 Third alternative design (AD3)

The block flow diagram for third alternative design (AD3) is shown in figure 3.10, it is like the base case design however both the CO_2 cleaning unit and WGS units have been removed

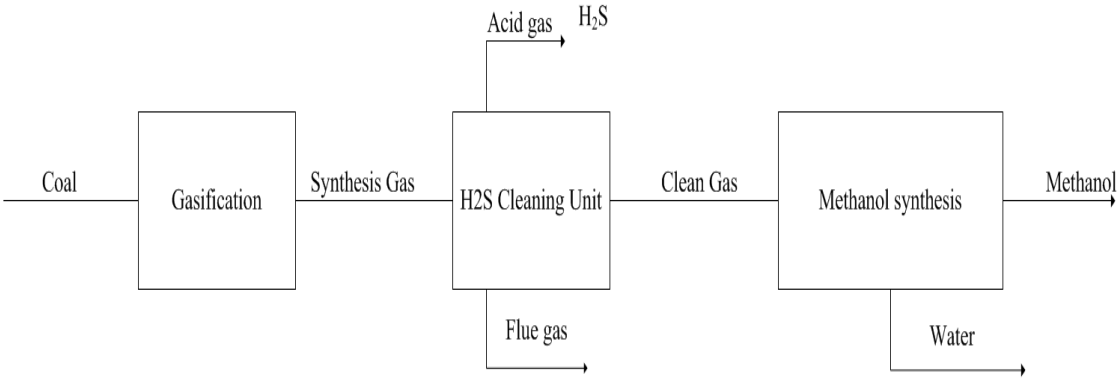

Figure 3-10: block flow diagram third alternative design

CHAPTER 4

PROCESS SIMULATION

This study builds the Methanol plant simulation models based on gasification with ASPEN PUS V.9 software. The details of model construction and parameters for the base case are described as follows.

4.1 Gasification unit

The feedstock to gasifier consists of water, coal and oxygen, while the output includes raw syngas and solid waste slag. The Gibbs reactor is used as gasifier to simulate the gasification process since it is reasonable to simulate the raw syngas with ideal thermodynamics when gasification reactions are at higher temperature [38]–[40].

For the simulation, the coal was characterized as coal bituminous and all of parameter of characterization set it as what have recorded in literature [41], [42] and illustrated in table 4-1 till table 4-4.. 100 thousand tons per year took as based feed. The coal mixed with 67.8 tons per hour before crushed and fed to the reactor. Oxygen have been used in the gasifier instated of Air, air separation unit have been used to have pure oxygen with purity 95 mol. percentage. The gasifier work at 32 bar and adiabatic condition the syngas left the gasifier with 1352 ^{o}C then it had been

cooled to 152 ^{o}C with heat recovery system and produce high pressure steam that can be used to generate electrical power.

Table 4-1: Proximate analysis of the bituminous Coal.

property	unit	value		
		Ash with moisture	Dry Base	Dry free Ash
Moisture content	wt.%	3.00	-	-
Ash content	wt.%	9.30	9.59	-
Volatile matter	wt.%	33.2	34.23	37.86
Fixed carbon	wt.%	54.49	56.18	62.14

Table 4-2: Ultimate analysis of the bituminous Coal.

property	unit	value		
		Ash with moisture	Dry Base	Dry free Ash
Carbon	wt.%	71.91	74.14	82.00
Hydrogen	wt.%	4.65	4.79	5.40
Nitrogen	wt.%	1.23	1.27	1.40
Sulphur	wt.%	0.35	0.36	0.40
Oxygen	wt.%	9.56	9.85	10.90
Total (with halides)	wt.%	100.00	100.00	100.00

Table 4-3: Calorific value of the bituminous Coal.

property	unit	value		
		Ash with moisture	Dry Base	Dry free Ash
Net calorific value (LHV)	MJ/kg	28.14	29.08	32.17
Gross calorific value (HHV)	MJ/kg	29.22	30.13	33.32
HHV $_{milne}$	MJ/kg	29.27	30.17	33.37

Table 4-4: Ash composition

property	unit	value
SO_3	wt.%	3.60
P_2O_5	wt.%	0.60
SiO_2	wt.%	40.80
Fe_2O_3	wt.%	4.80
Al_2O_3	wt.%	31.10
CaO	wt.%	7.40
MgO	wt.%	2.10
Na_2O	wt.%	1.00
K_2O	wt.%	1.10
TiO_2	wt.%	1.50

Figure 4-1, figure 4-2 and figure 4-3 shows this process as it had been simulated in ASPEN PLUS .

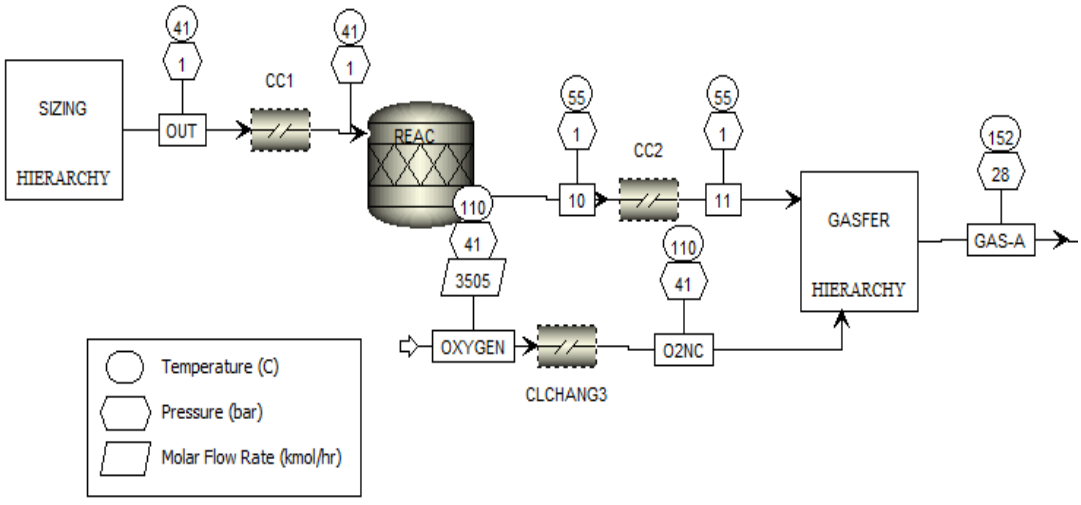

Figure 4-1: simulation of the overall gasification process.

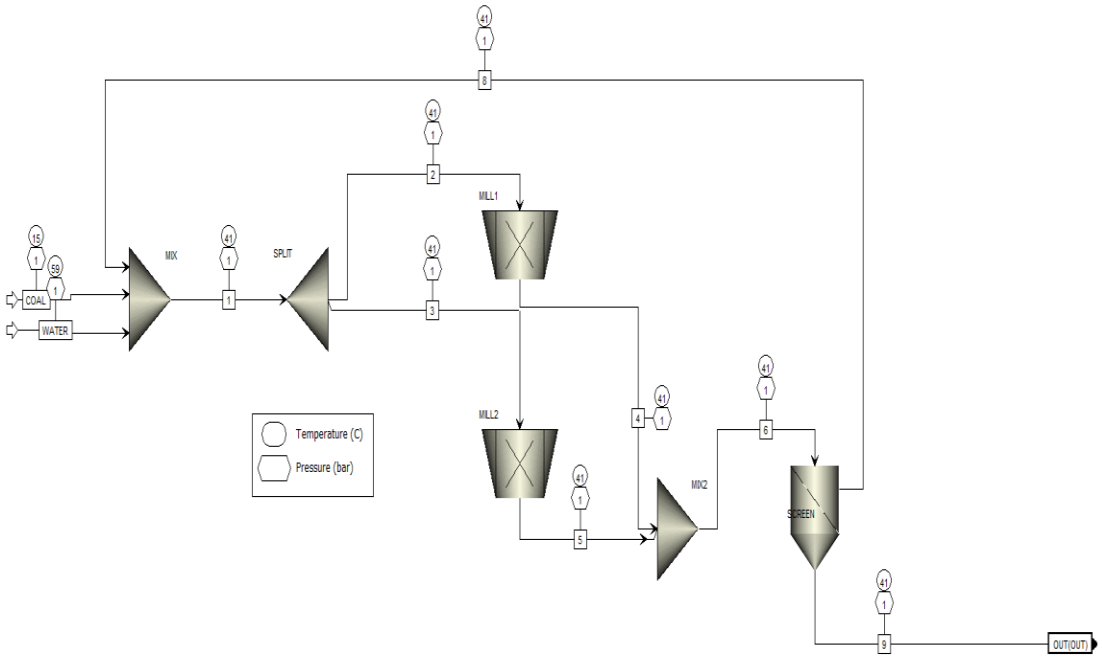

Figure 4-2: Feed preparation simulation.

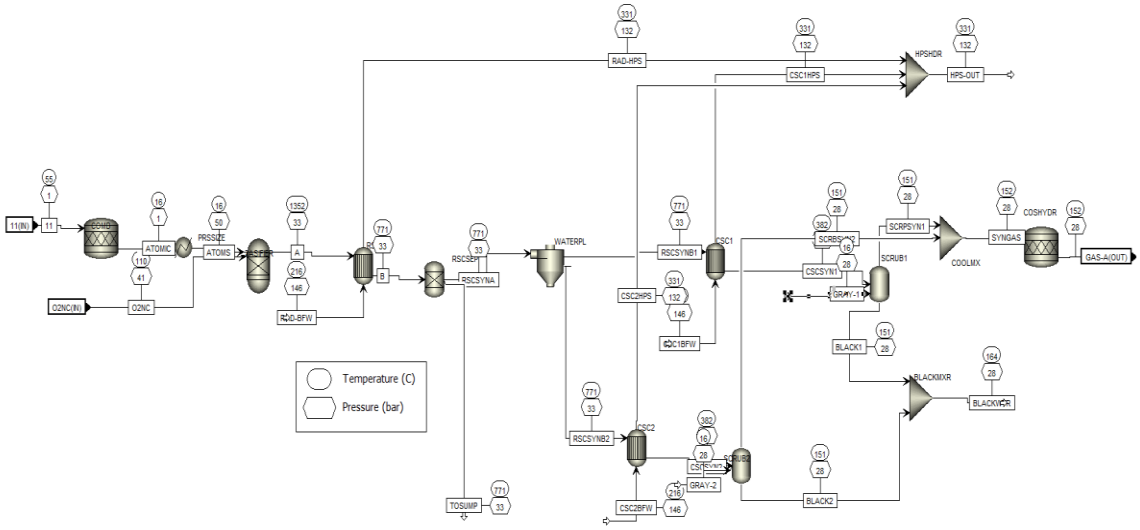

Figure 4-3: Simulation for Gasifier and steam generation part.

4.2 Acid gas removal unit

The row syngas has been treated two absorbers in series that designed to remove almost all the acid gas from the feed the first absorber that removed H_2S consist of 20 equilibrium stages while the second column for removing CO_2 consist from 10 equilibrium stages. The solvent flow rate optimized to remove all the acid gas with minimum consumption of the solvent. The rich solvent fed to seven stages in the stripper that contains 10 equilibrium stages with reflux ratio equal to one and the bottom product is lean solvent can be recycled to absorber column.

Figure 4-4 and figure 4-5 shows the simulation for the cleaning unit.

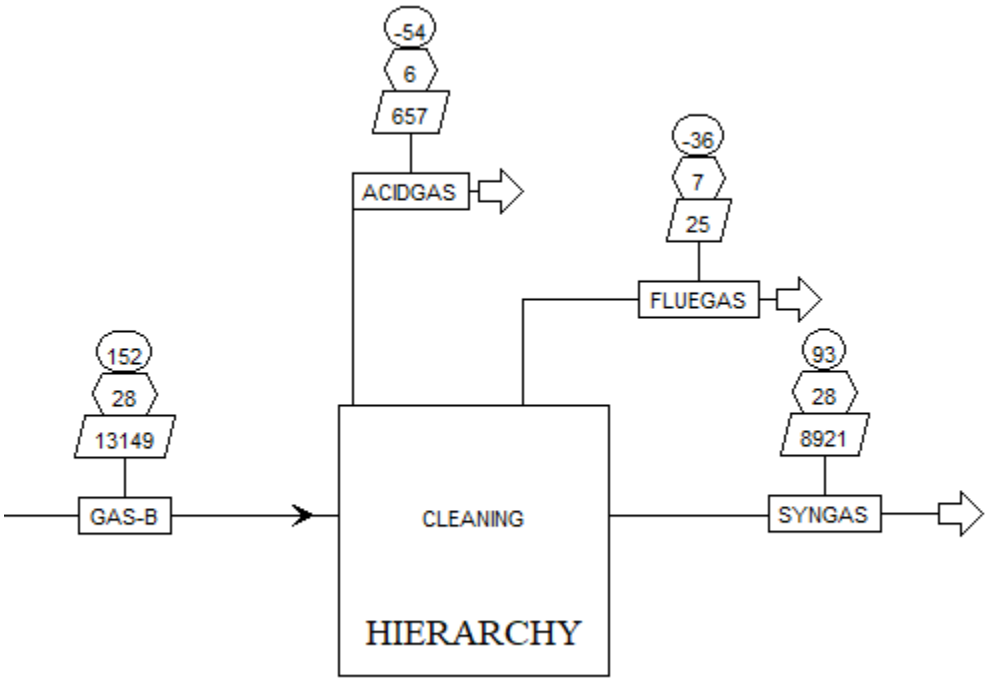

Figure 4-4:Simulation of the overall acid gas removal unit.

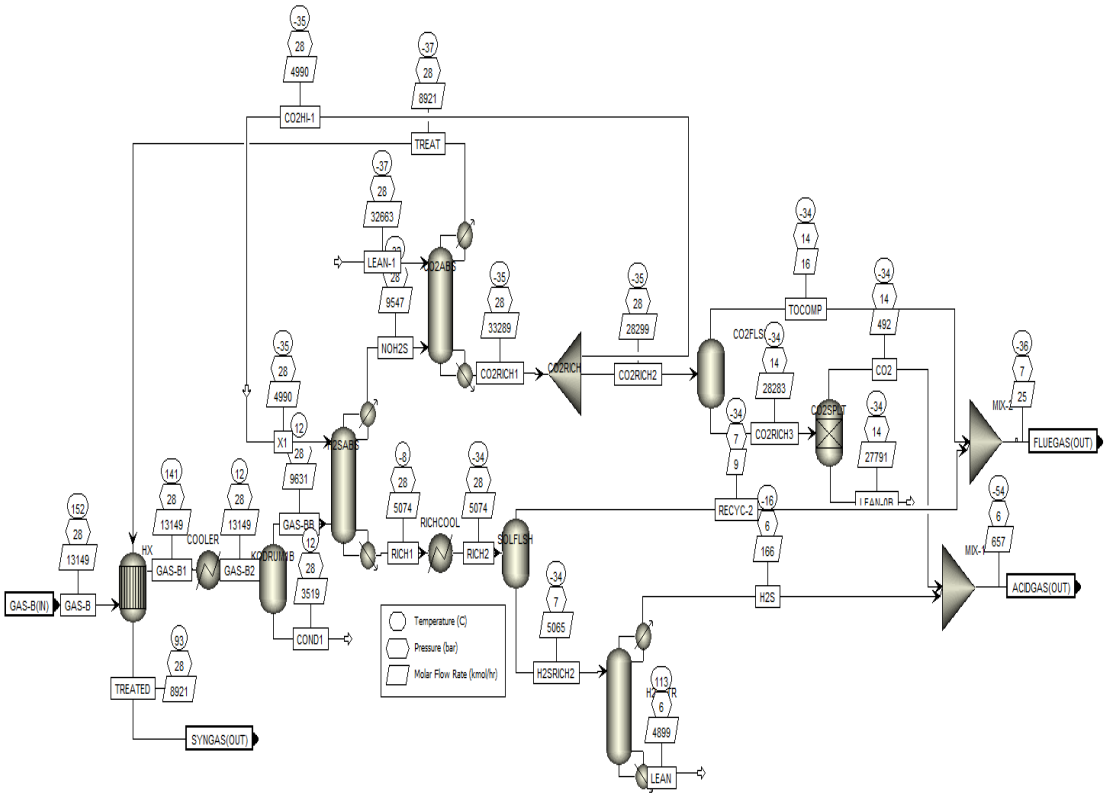

Figure 4-5: Simulation of Cleaning unit.

4.3 Water gas shift unit

This unit contains two equilibrium reactors with intercooling work under adiabatic condition the syngas converted through equation 2-13 to hydrogen and carbon dioxide. The amount of steam has been optimized to give high amount of hydrogen by studding the sensitivity analysis for hydrogen produced with respects to amount of steam needs. The ratio of CO_2 to H_2 was manipulated using Carbon dioxide capture unit (CCU) that used physical solvent (methanol) in absorber column contains 15 equilibrium stages and it equals to three.

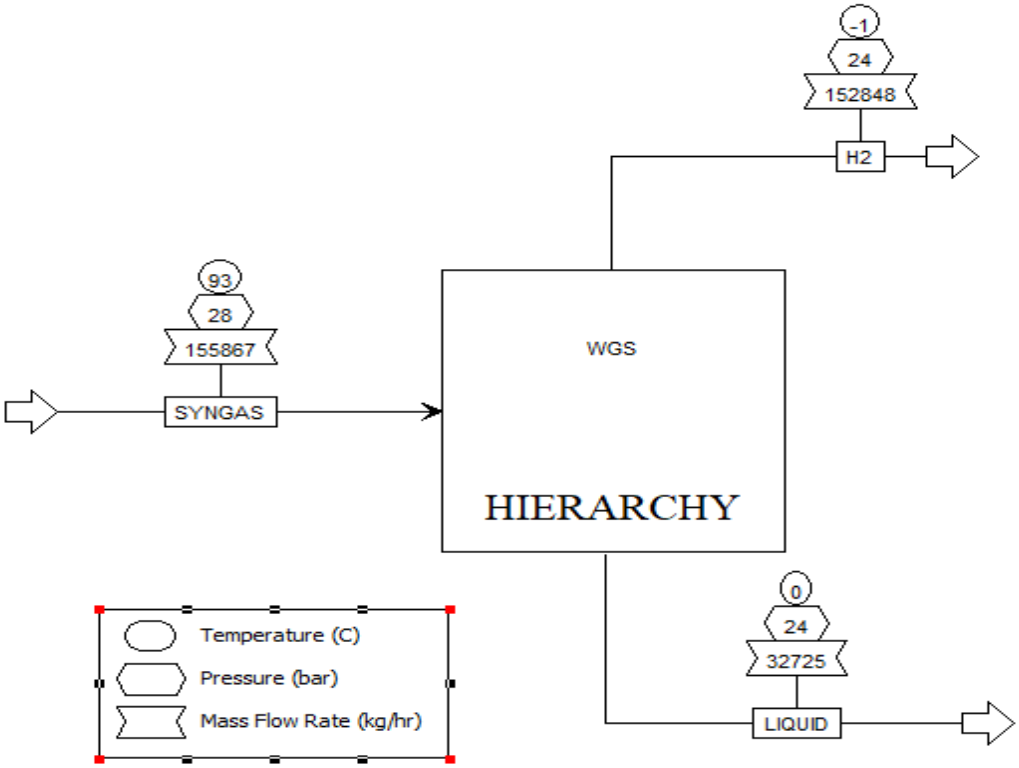

Figure 4-6: simulation of the overall WGS unit.

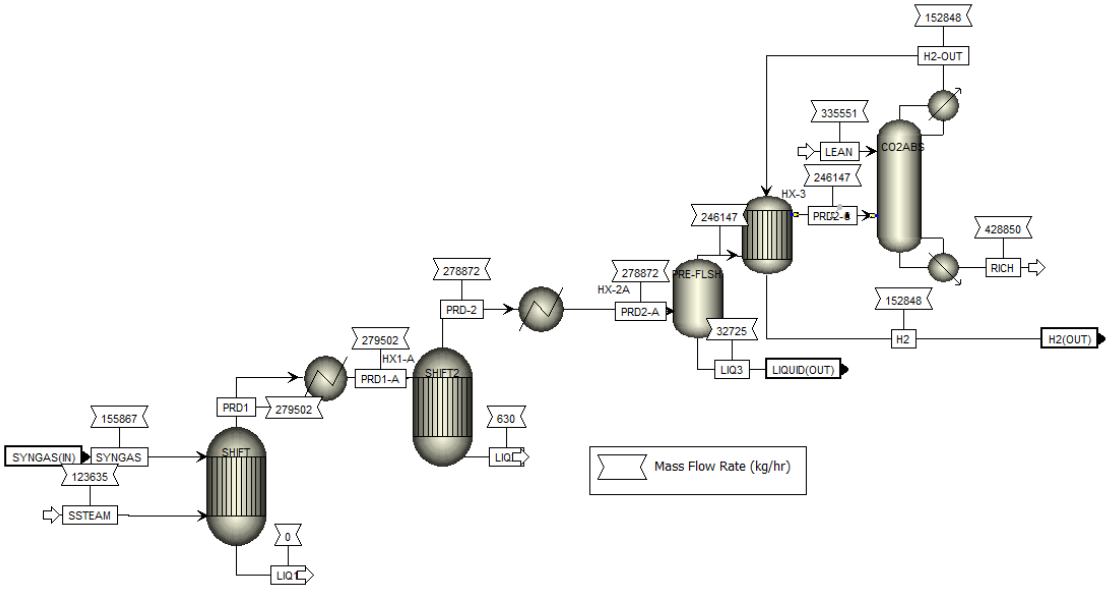

Figure 4-7: Simulation for WGS unit.

4.4 Methanol synthesis unit

The benchmark model adopts clean syngas as feedstock. First, the pressure and temperature of syngas are increased to 78 bars and 210 ^{o}C. by compressor and heat exchanger, respectively. Then, syngas is fed to adiabatic fixed bed reactor with to product methanol. The kinetic model used in this paper is that of Vanden Bussche and Froment (1996) with readjusted parameters of Mignard and Pritchard (2008) (Equation 4-1 and 4-2, in which pressures are expressed in bar and temperatures in K). The kinetic constants follow the Arrhenius law (Equation 4-3), its parameters are shown in table 4-5. Graaf et al. (1986) give the thermodynamic equilibrium constants (Equation 4-4 and 4-5) that are described below[11], [43]–[45].

$$r_{CH_3OH} = \frac{k_1 P_{CO_2} P_{H_2} \left(1 - \frac{1}{K_1} \frac{P_{H_2O} P_{CH_3OH}}{P_{H_2}^{\ 3} P_{CO_2}}\right)}{\left(1 + k_2 \frac{P_{H_2O}}{P_{H_2}} + k_3 P_{H_2}^{\ 0.5} + k_4 P_{H_2O}\right)^3} \qquad \left[\frac{mol}{Kg_{cat} \cdot S}\right] \qquad (4\text{-}1)$$

$$r_{RWGS} = \frac{k_5 P_{CO_2} P_{H_2} \left(1 - \frac{1}{K_2} \frac{P_{H_2O} P_{CO}}{P_{CO_2} P_{H_2}}\right)}{\left(1 + k_2 \frac{P_{H_2O}}{P_{H_2}} + k_3 P_{H_2}^{\ 0.5} + k_4 P_{H_2O}\right)} \qquad \left[\frac{mol}{Kg_{cat} \cdot S}\right] \qquad (4\text{-}2)$$

$$k_i = A_i \exp\left(\frac{B_i}{R\,T}\right) \qquad (4\text{-}3)$$

$$\log K_1 = \frac{3066}{T} - 10.592 \qquad (4\text{-}4)$$

$$\log K_2 = 2.029 - \frac{2073}{T} \tag{4-5}$$

The outlet gas goes through the purification processes that consist from two stages firstly is low pressure flash separator then it fed into the 14 stage of distillation column contains 19 stages as total with 0.87 reflux ratio to produce 98.7 wt.% purity methanol.

Table 4-5: Parameters values for the kinetic model[11].

k1	A_1	1.07
	B_1	40,000
k2	A_2	3,453.38
	B_2	-
k3	A_3	0.499
	B_3	17,197
k4	A_4	$6.62 * 10^{-11}$
	B_4	124,119
k5	A_5	$1.22 * 10^{10}$
	B_5	-98,084

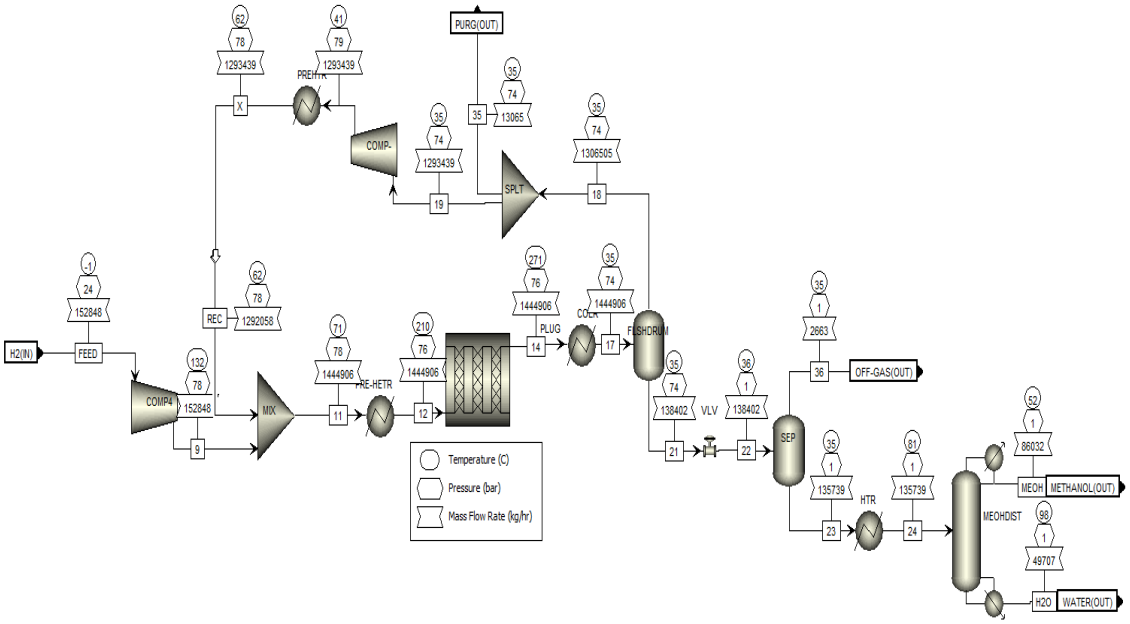

Figure 4-8: Simulation of Methanol Synthesis Unit.

CHAPTER 5

RESULTS AND DISCUSSION

5.1 Stream Result

The main streams in the flow sheet result mention in the following section for the base case and the alternatives design.

5.1.1 Base case

The result for the first three units are gasification, acid gas removal and WGS are shown in table 5-1 and the methanol synthesis in table 5-2.

Table 5-1: Base case Stream results for gasification, AGR and WGS.

	units	***Syngas produce***	***sweet Syngas***	***acid gas removed***	***Flue Gas***	***Produced gas***
Temp	***°C***	152.5	93.3	-54.4	-35.6	-1.2
pressure	***bar***	27.6	27.6	5.5	6.9	24.1
mass flow	***kg/hr***	273749.0	155867.0	27795.5	602.0	152848.0
mole flow	***kmol/hr***	13149.2	8921.1	657.2	24.9	11805.7
composition		***mole fraction***				
N_2		0.0089	0.0125	0.0035	0.0231	0.0094
AR		0.0091	0.0126	0.0060	0.0254	0.0094
H_2O		0.1902	0.0000	0.0000	0.0000	0.0000
CO		0.3931	0.5636	0.0289	0.6606	0.0015
CO_2		0.1153	0.0000	0.8579	0.0793	0.2448
H_2S		0.0035	0.0000	0.0555	0.0018	0.0000
H_2		0.2795	0.4112	0.0023	0.2092	0.7345
MEOH		0.0000	0.0001	0.0427	0.0003	0.0003
Total		1.000	1.000	0.997	1.000	1.000

Table 5-2:Base case Methanol synthesis streams result.

	units	***Feed***	***To reactor***	***product***	***Purge***	***Off Gas***	***Methanol***	***water***
Temp	***°C***	-1.2	210.0	271.0	35.0	35.0	52.1	97.7
pressure	***Bar***	24.1	76.4	75.9	74.3	1.2	1.0	1.0
mass flow	***kg/hr***	152848.0	1444906.5	1444906.5	13065.0	2663.2	86031.8	49707.0
mole flow	***kmol/hr***	11805.7	94395.1	88982.1	834.9	67.4	2703.0	2723.4
composition		***mole fraction***						
N_2		0.0094	0.0964	0.1023	0.1090	0.0221	0.0000	0.0000
AR		0.0094	0.0940	0.0997	0.1062	0.0649	0.0000	0.0000
H_2O		0.0000	0.0005	0.0312	0.0006	0.0265	0.0170	0.9831
CO		0.0015	0.0356	0.0380	0.0405	0.0042	0.0000	0.0000
CO_2		0.2448	0.1474	0.1258	0.1334	0.7162	0.0021	0.0000
H_2S		0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
H_2		0.7345	0.6227	0.5691	0.6065	0.0372	0.0000	0.0000
MEOH		0.0003	0.0030	0.0336	0.0034	0.1287	0.9809	0.0169
Total		1.000	1.000	1.000	1.000	1.000	1.000	1.000

Table 5-3: Base case PFR parameter and the stoichiometry number.

Conversion =	19.6 %
SN =	2.0

5.1.2 First alternative design

Table 5-4: AD1 Stream results for gasification, AGR and WGS.

	units	***Syngas produce***	***sweet Syngas***	***H2S removed***	***Flue Gas***	***Produced gas***
Temp	***°C***	152.5	-29.6	15.0	-33.7	-1.2
pressure	***bar***	27.6	27.6	5.5	6.9	24.1
mass flow	***Kg/hr***	273749.0	181159.6	4386.9	175.4	153733.0
mole flow	***kmol/hr***	13149.2	9514.7	108.9	6.9	11858.6
composition		***mole fraction***				
N_2		0.0089	0.0121	0.0017	0.0267	0.0096
AR		0.0091	0.0122	0.0030	0.0316	0.0096
H_2O		0.1902	0.0000	0.0000	0.0000	0.0000
CO		0.3931	0.5317	0.0112	0.6512	0.0019
CO_2		0.1153	0.0574	0.6338	0.1069	0.2446
H_2S		0.0035	0.0001	0.3267	0.0072	0.0000
H_2		0.2795	0.3861	0.0007	0.1756	0.7339
MEOH		0.0000	0.0002	0.0162	0.0004	0.0003
Total		1.000	1.000	0.993	1.000	1.000

Table 5-5: AD1 Methanol synthesis streams result.

	units	***Feed***	***To reactor***	***product***	***Purge***	***Off-Gas***	***Methanol***	***water***
Temp	***°C***	-1	410	520	35	35	52	96
pressure	***bar***	24	1108	1108	74	1	1	1
mass flow	***Kg/hr***	153733	3277891	3277891	13476	2735	85654	50796
mole flow	***kmol/hr***	11859	210785	198782	846	69		
composition		***mole fraction***						
N_2		0.010	0.098	0.104	0.111	0.022	0.000	0.000
AR		0.010	0.097	0.102	0.109	0.065	0.000	0.000
H_2O		0.000	0.001	0.031	0.001	0.026	0.017	0.974
CO		0.002	0.036	0.039	0.041	0.004	0.000	0.000
CO_2		0.245	0.150	0.128	0.136	0.716	0.002	0.000
H_2S		0.000	0.000	0.000	0.000	0.000	0.000	0.000
H_2		0.734	0.616	0.562	0.599	0.036	0.000	0.000
MEOH		0.000	0.003	0.033	0.003	0.129	0.981	0.026
Total		1.000	1.000	1.000	1.000	0.999	1.000	1.000

Table 5-6: AD1 PFR parameter and the stoichiometry number.

Conversion =	19.2	%
SN =	2.0	

5.1.3 Second alternative design

Table 5-7: AD2 Stream results for gasification, AGR and WGS.

	units	***Syngas produce***	***sweet Syngas***	***H2S removed***	***Flue Gas***	***Produced gas***
Temp	***°C***	152.5	-29.6	15.0	-33.7	c
pressure	***bar***	27.6	27.6	5.5	6.9	24.1
mass flow	***Kg/hr***	273749.0	181159.6	4386.9	175.4	271899.0
mole flow	***kmol/hr***	13149.2	9514.7	108.9	6.9	14553.0
composition		***mole fraction***				
N_2		0.0089	0.0121	0.0017	0.0267	0.0079
AR		0.0091	0.0122	0.0030	0.0316	0.0080
H_2O		0.1902	0.0000	0.0000	0.0000	0.0002
CO		0.3931	0.5317	0.0112	0.6512	0.0016
CO_2		0.1153	0.0574	0.6338	0.1069	0.3836
H_2S		0.0035	0.0001	0.3267	0.0072	0.0001
H_2		0.2795	0.3861	0.0007	0.1756	0.5985
MEOH		0.0000	0.0002	0.0162	0.0004	0.0000
Total		1.000	1.000	0.993	1.000	1.000

Table 5-8: AD2 Methanol synthesis streams result.

	units	Feed	Fresh hydrogen	comp Mix feed	To reactor	product	Purge	Off Gas
Temp	°C	0.0	25.0	135.9	210.0	271.0	35.0	35.0
pressure	bar	24.1	30.0	78.0	76.4	76.4	74.3	1.2
mass flow	Kg/hr	271889.0	16202.9	288101.0	2573170.6	2573170.6	23082.9	5172.2
mole flow	kmol/hr	14553.0	8037.6	22590.6	200899.0	190568.0	1800.4	130.5
composition		mole fraction						
N_2		0.008	0.000	0.005	0.047	0.050	0.053	0.010
AR		0.008	0.000	0.005	0.047	0.049	0.052	0.031
H_2O		0.000	0.000	0.000	0.001	0.028	0.001	0.027
CO		0.002	0.000	0.001	0.049	0.053	0.056	0.006
CO_2		0.384	0.000	0.247	0.153	0.133	0.140	0.753
H_2S		0.000	0.000	0.000	0.000	0.000	0.000	0.000
H_2		0.599	1.000	0.741	0.700	0.657	0.695	0.042
MEOH		0.000	0.000	0.000	0.003	0.030	0.003	0.128
Total		1.000	1.000	1.000	1.000	1.000	1.000	0.997

Table 5-9: AD2 Stream result for product of Methanol synthesis.

	units	***Methanol***	***water***
Temp	***°C***	51.8	94.4
pressure	***bar***	1.0	1.0
mass flow	***Kg/hr***	160854.0	98849.80
mole flow	***kmol/hr***	5050.7	5344.21
composition		***mole fraction***	
N2		0.000	0.000
AR		0.000	0.000
H2O		0.016	0.966
CO		0.000	0.000
CO2		0.002	0.000
H2S		0.000	0.000
H2		0.000	0.000
MEOH		0.982	0.034
Total		1.000	1.000

Table 5-10: AD2 PFR parameter and the stoichiometry number.

Conversion =	17.1	%
SN =	2.0	

5.1.4 Third alternative design

Table 5-11: AD3 Stream results for gasification and AGR.

	units	Syngas produce	sweet Syngas	H2S removed	Flue Gas
Temp	°C	152.5	-29.6	15.0	-33.7
pressure	bar	27.6	27.6	5.5	6.9
mass flow	Kg/hr	273749.0	181159.6	4386.9	175.4
mole flow	kmol/hr	13149.2	9514.7	108.9	6.9
composition		mole fraction			
N2		0.0089	0.0121	0.0017	0.0267
AR		0.0091	0.0122	0.0030	0.0316
H2O		0.1902	0.0000	0.0000	0.0000
CO		0.3931	0.5317	0.0112	0.6512
CO2		0.1153	0.0574	0.6338	0.1069
H2S		0.0035	0.0001	0.3267	0.0072
H2		0.2795	0.3861	0.0007	0.1756
MEOH		0.0000	0.0002	0.0162	0.0004
Total		1.000	1.000	0.993	1.000

Table 5-12: AD3 Methanol synthesis streams result.

	units	Feed	To reactor	Product	Purge	Off-Gas	Methanol	water
Temp	°C	-29.6	210	271	35	35.0	22.9	68.3
pressure	bar	27.6	76.4	75.9	74.3	1.2	1.0	1.0
mass flow	Kg/hr	181159.6	11550392.29	11550392.29	114928.9	4212.8	49592.4	3700.9
mole flow	kmol/hr	9514.7	409245.18	405874.12	4040.9	109.0	1546.5	129.4
composition		mole fraction						
N2		0.012	0.027	0.027	0.027	0.011	0.000	0.000
AR		0.012	0.027	0.027	0.027	0.016	0.000	0.000
H2O		0.000	0.000	0.000	0.000	0.002	0.003	0.245
CO		0.532	0.766	0.768	0.772	0.135	0.000	0.000
CO2		0.057	0.103	0.104	0.104	0.601	0.006	0.000
H2S		0.000	0.000	0.000	0.000	0.004	0.000	0.000
H2		0.386	0.069	0.061	0.061	0.004	0.000	0.000
MEOH		0.000	0.007	0.011	0.007	0.224	0.991	0.755
Total		1.000	0.999	1.000	1.000	0.997	1.000	1.000

Table 5-13: AD3 PFR parameter and the stoichiometry number.

Conversion =	0.09 %
SN =	0.56

5.2 Energy Analysis and performance

To have a fare comparison between all cases energy consumption per production rate is on scenario to compare it. Figure 5-1 illustrate that alternative design 2 has the least energy consumption comparable to other cases with 9.2 M.hr/tons. While the base case and alternative design 1 has the same energy consumption with 11.8 MW.hr/tons. However, the alternative design 2 has the worst case with higher energy consumption 44 MW.hr/tons.

The energy distribution between all the units in each case have been shown in figure 5-2. Methanol section has the higher contribution in energy consumption in the plant while the cleaning unit has the less contribution. However, the gasification and water gas shift unit have moderate consumption.

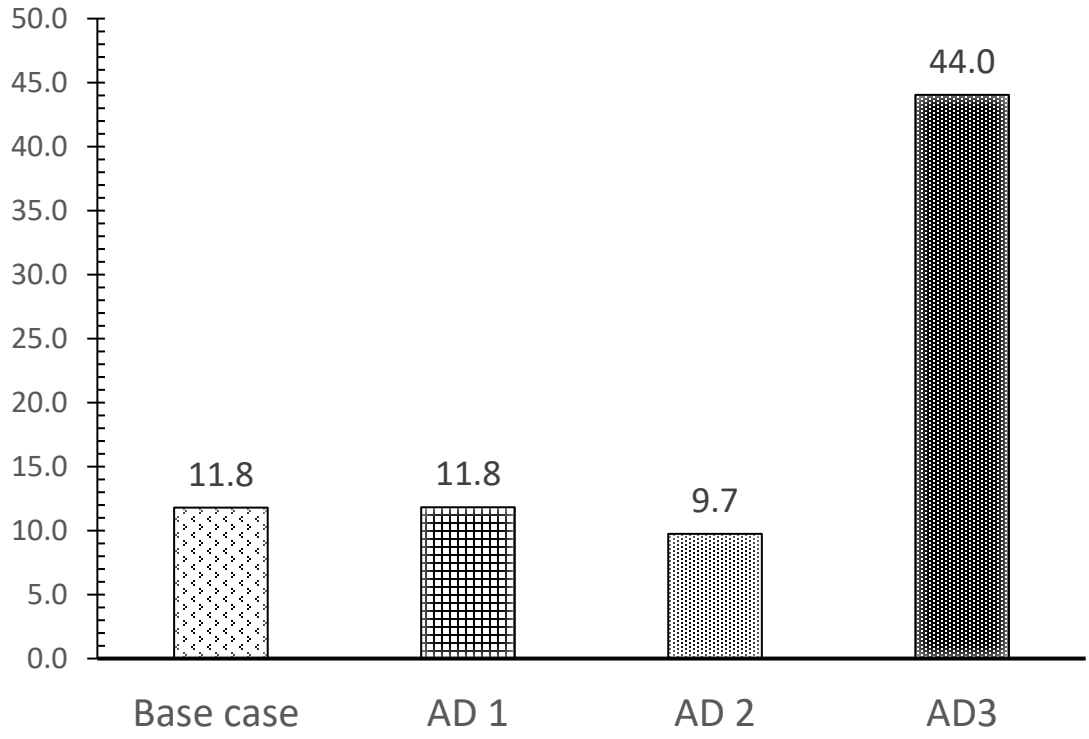

Figure 5-1: Energy consumption per production rate.

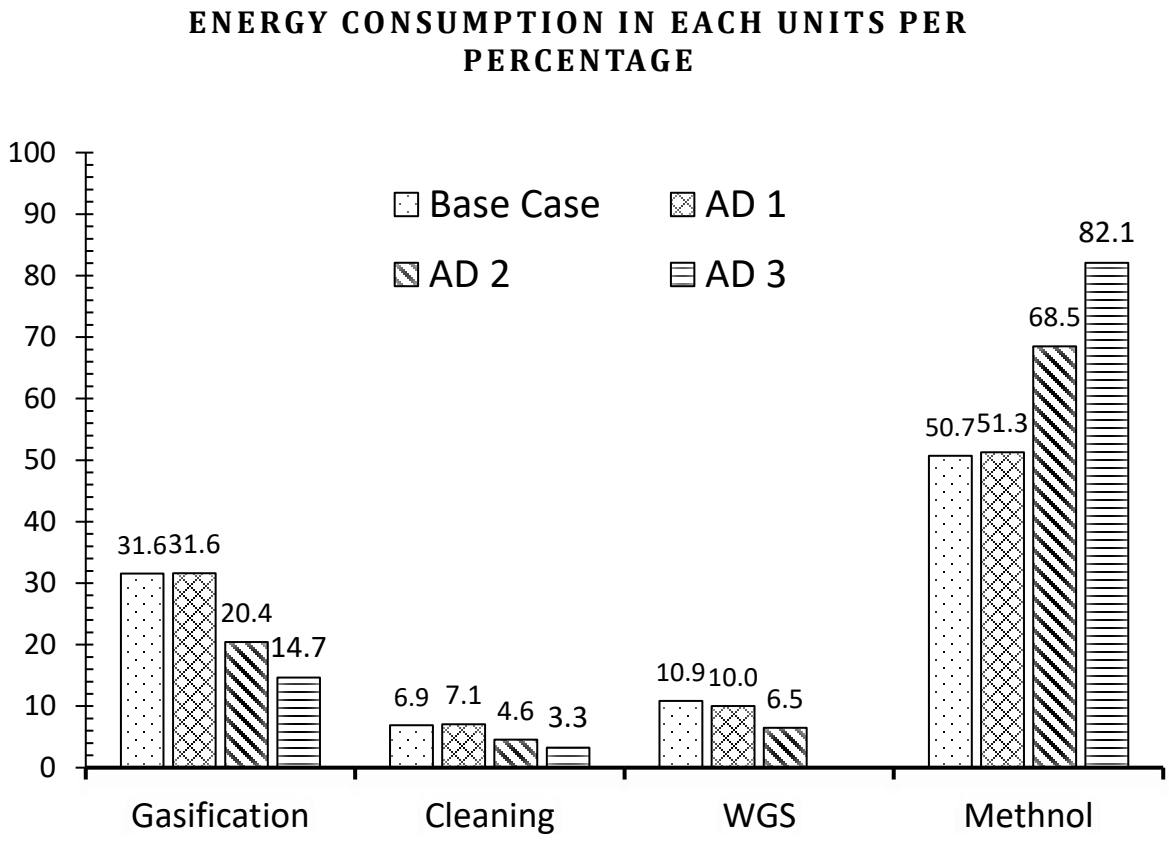

Figure 5-2: Energy consumption percentage for each unit.

5.3 Carbon dioxide emission

Carbon dioxide emission: One of the main parameter to compare between processes is CO_2 emission. it occurs in three different ways in the process are CO_2 rejected from: cleaning unit, WGS unit and methanol synthesis unit. The details are as shown in figure 5-3.

Alternative Design 2 shows that it has the less emission of CO_2 that equals to almost 90 tons of CO_2 per year while alternative design three has moderate emission. However, the bas e case and alternative design 1 have almost same emission that is around 570 tons of CO_2 per year.

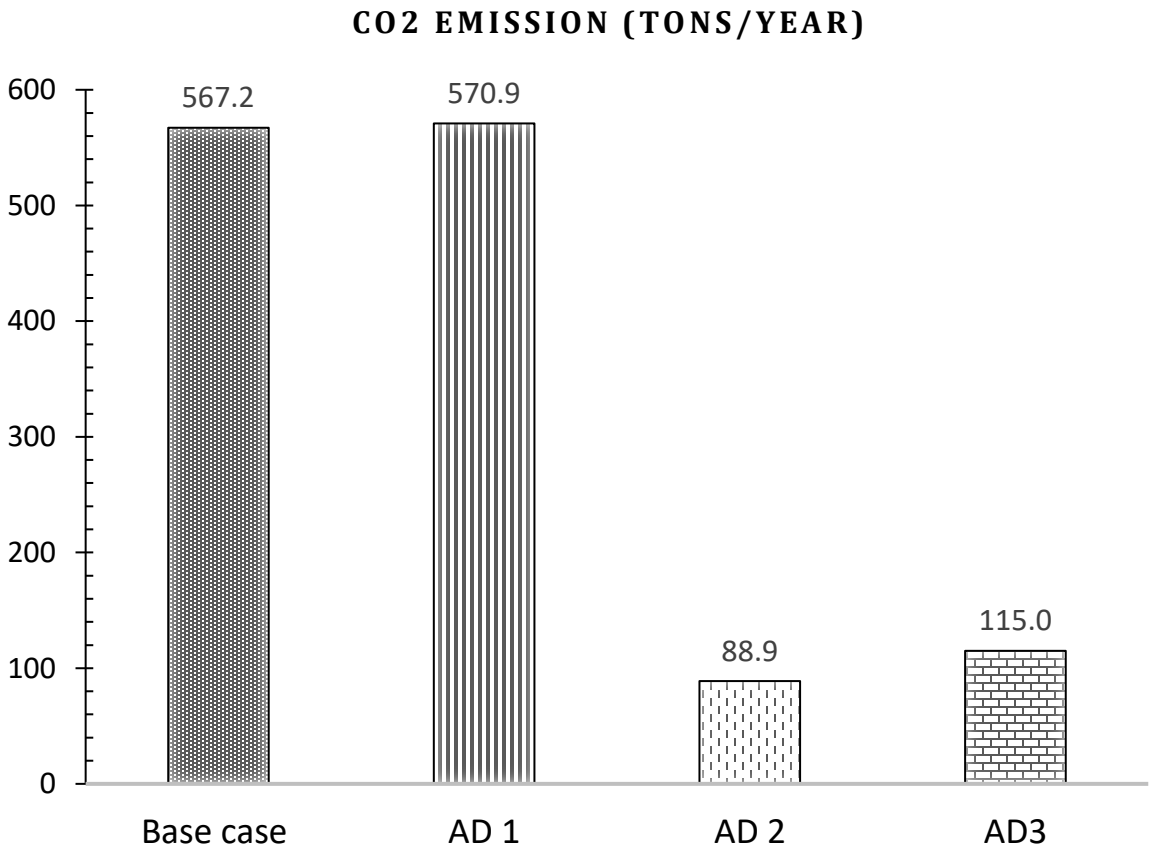

Figure 5-3: CO_2 emission

5.4 Cost analysis

5.4.1 Capital cost:

Capital cost has been calculated using Aspen Plus Economics and the missing data calculated using Cap-cost the result recorded in figure 5-4 below. Figure 5-4 shows that the Base case has lower capital cost while AD 3 has the higher capital cost due to the large recycle streams amount therefor the size of equipment has large comparable to lower recycle flow rate. However, the Alternative Design 2 and 3 has moderate recycle stream amount that it has moderate cost.

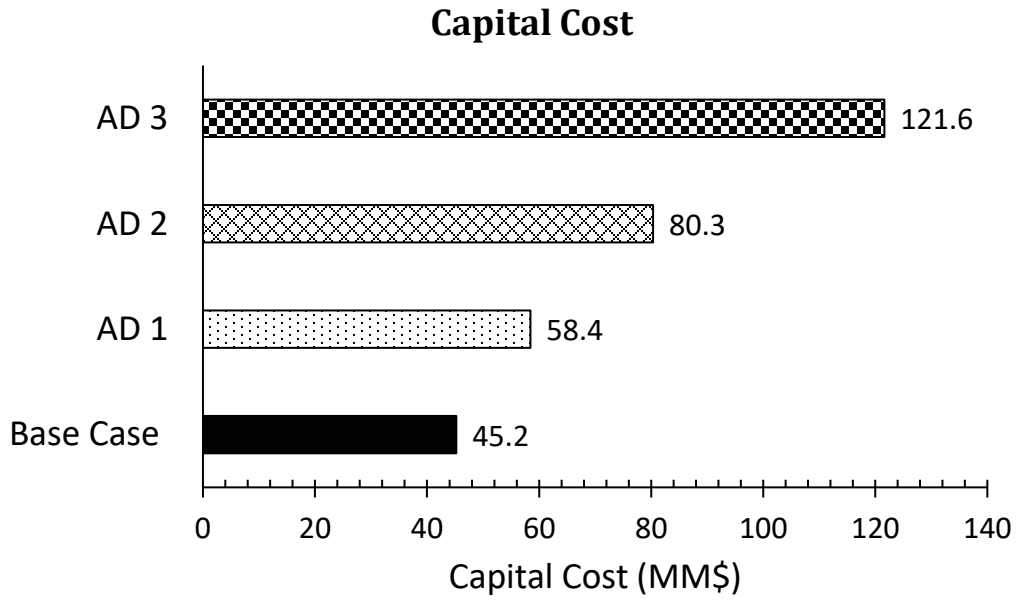

Figure 5-4: Capital Cost for the cases.

5.4.2 Operation cost:

Operation cost have been calculated using Aspen Plus Economics and the result recorded in figure 5-5 below. As it mentions early the recycle stream and feed amount effects the size of equipment there for effect the energy of equipment's there for it leads to have high operation cost.

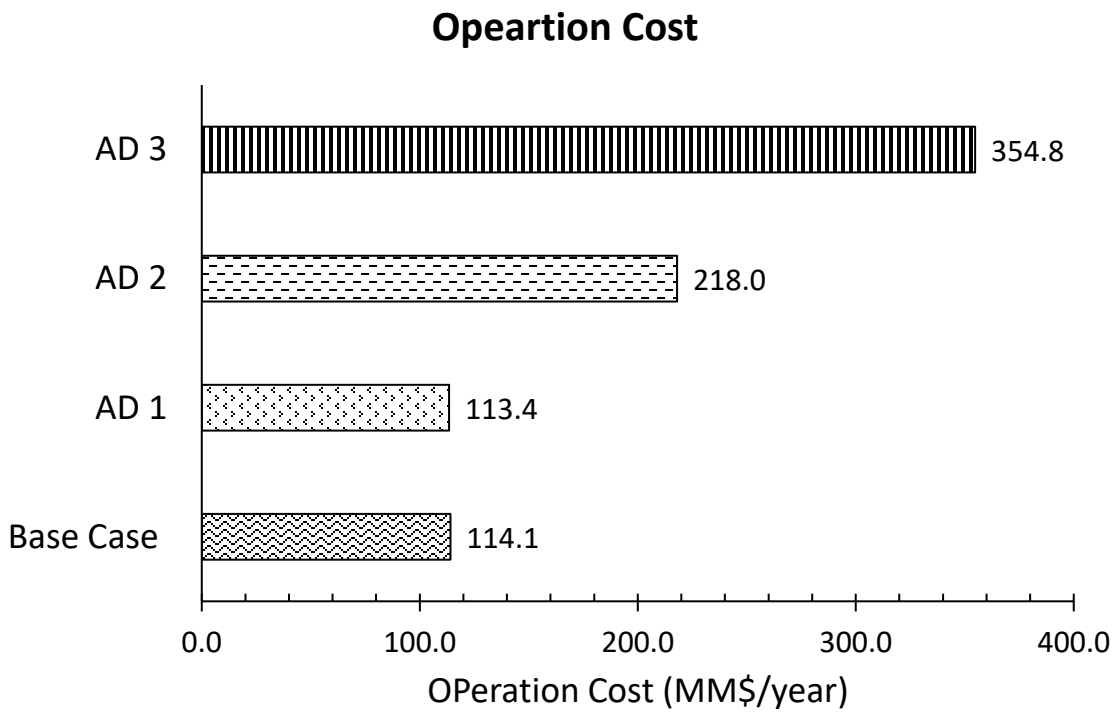

Figure 5-5: Operation Cost for all Cases.

5.4.3 Cost of unit produced

To have a fare base to compare between the cases this parameter is most important. Figure 5-6 illustrate the cost to produce a ton of methanol assuming that the life time for the project is 20 years and the interest factor is 10%. Figure 5-6 shows the base case and alternative design 1 and 2 have almost same cost for production tons of methanol which around 165 $/ton while alternative design 3 has more expensive cost due to low conversion of Carbon dioxide.

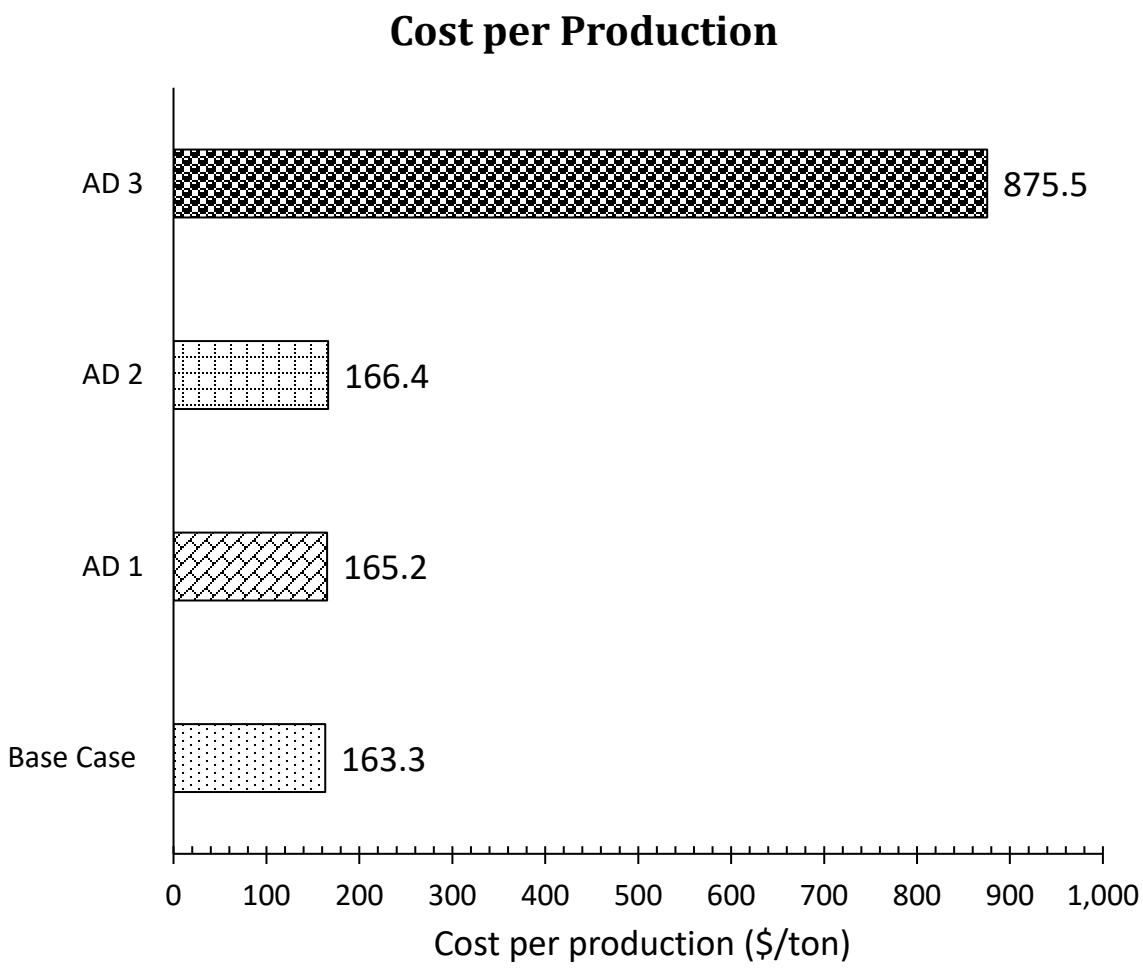

Figure 5-6: Cost per production of methanol.

CHAPTER 6

CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusion

The conversion of coal to methanol process with ASPEN PLUS simulation model has been performed. The four major processes include gasification process, gas clean-up modules, water gas shift unit and methanol synthetic unit. The simulation procedures are performed in a case study of methanol production. Three alternative design have been developed to enhance the performance of the process.

The result shows that the methanol synthesis from coal through gasification technology is feasible. The second alternative design shows it has best performance in terms of energy consumption, CO2 emission and it in the same range in the cost per production and have value of 9.7 MW.hr/ton Methanol, 88.9-ton CO_2 /year and 166.4 $/ton methanol respectively.

6.2 Recommendation

- This study can be improved by further research work to optimize the the energy consumption in the methanol synthesis section because it has the higher consumption of the energy.
- Study the effect of using different type of feedstock for the gasification section as example use the bio-mass or the vacuumed residue (VR) from the vacuum distillation column because it has lower carbon content and the VR can produce higher hydrogen when it gasified.
- Study the sensitivity analysis for the main parameters that effect the process performance.
- Study the effect of using different type of solvent for the cleaning unit.

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